MULTIPLE-FLAME COMBUSTION MODEL FORTRAN IV COMPUTER PROGRAM

G. D. Sammons, et al

Rockwell International Corporation

Prepared for:

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Several investigators have formulated competing-flame models discribing composite solid propellant combustion. This report covers Mr G D Sammons' (deceased) competing-flame modeling efforts. His papers describing the model are appended. This report describes and lists the FORTRAN IV computer program which is the practical outcome of any modeling effort. Included is the solution of an example of problem--estimation of the burn rate of a low-smoke HTPB propellant. How the necessary input values are obtained and how they are input is discussed in detail. Finally, the computer solution printout is depicted. The work described here was performed under sponsorship of the Combustion Energetics Division of the Air Force Office of Scientific Research (Contract F44620-72-C-0045).

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SCIENTIFIC REPORT

MULTIPLE-FLAME COMBUSTION MODEL

FORTRAN IV COMPUTER PROGRAM

FINAL

Submitted to Combustion Energetics Division, AFOSR

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Work performed under sponsorship of the Combustion Energetics Division of the Air Force Office of Scientific Research, Contract F44620-72-C-0046

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FOREWORD

This report consists of a User's Guide and Fortran IV source deck for G. D. Sammons' (deceased) Combustion Model Computer Program written under paragraph A.I.3 of Item 0001 in Contract F44620-72-C-0046. This report was assembled for publication by members of the Technical Staff, Rocketdyne, McGregor, Texas. Lloyd R. Lawrence, Jr., Captain USAF, from the Air Force Office of Scientific Research, was monitor for the program.

SCIENTIFIC REPORT
MULTIPLE-FLAME COMBUSTION MODEL
FORTRAN IV COMPUTER PROGRAM

ABSTRACT

Several investigators have formulated competing-flame models describing composite solid propellant combustion. This report covers Mr. G. D. Sammons' (deceased) competing-flame modeling efforts. His papers describing the model are appended. This report describes and lists the FORTRAN IV computer program which is the practical outcome of any modeling effort. Included is the solution of an example problem--estimation of the burning rate of a low-smoke HTPB propellant. How the necessary input values are obtained and how they are input is discussed in detail. Finally, the computer solution printout is depicted.

The work described here was performed under sponsorship of the Combustion Energetics Division of the Air Force Office of Scientific Research (Contract F44620-72-C-0046).

Combustion modeling studies will be continued during FY 1975. These further studies will be directed primarily toward addition of a mathematical treatment for heterogeneous catalysis of burning rate to the multiple-flame model.

CONTENTS

INTRODUCTION

Considerable efforts over the past seventeen years have been directed toward elucidating the mechanism of combustion of composite solid propellants. The ultimate goal of these efforts has been a truly comprehensive and descriptive mathematical combustion model. The most sophisticated models stemming from these efforts are the competing-flame models of Hermance[1][2] and Beckstead, Derr and Price (BDP)[3][4]. These combustion models allow one to use some independently determined kinetic and thermal parameters to predict burning rate. This report covers one of the more recent modeling efforts--Mr. G. D. Sammons' (deceased) extension of the BDP competing-flame model.

Mr. Sammons' papers presented at the 9th and 10th JANNAF Combustion Meetings, which describe his model, are appended to this report as Appendix I. His computer program originally written in FORTRAN IV for use at a time-share computer terminal has been rewritten for use on an IBM-360. This rewritten program is described here briefly. Also given here is a solved sample problem.

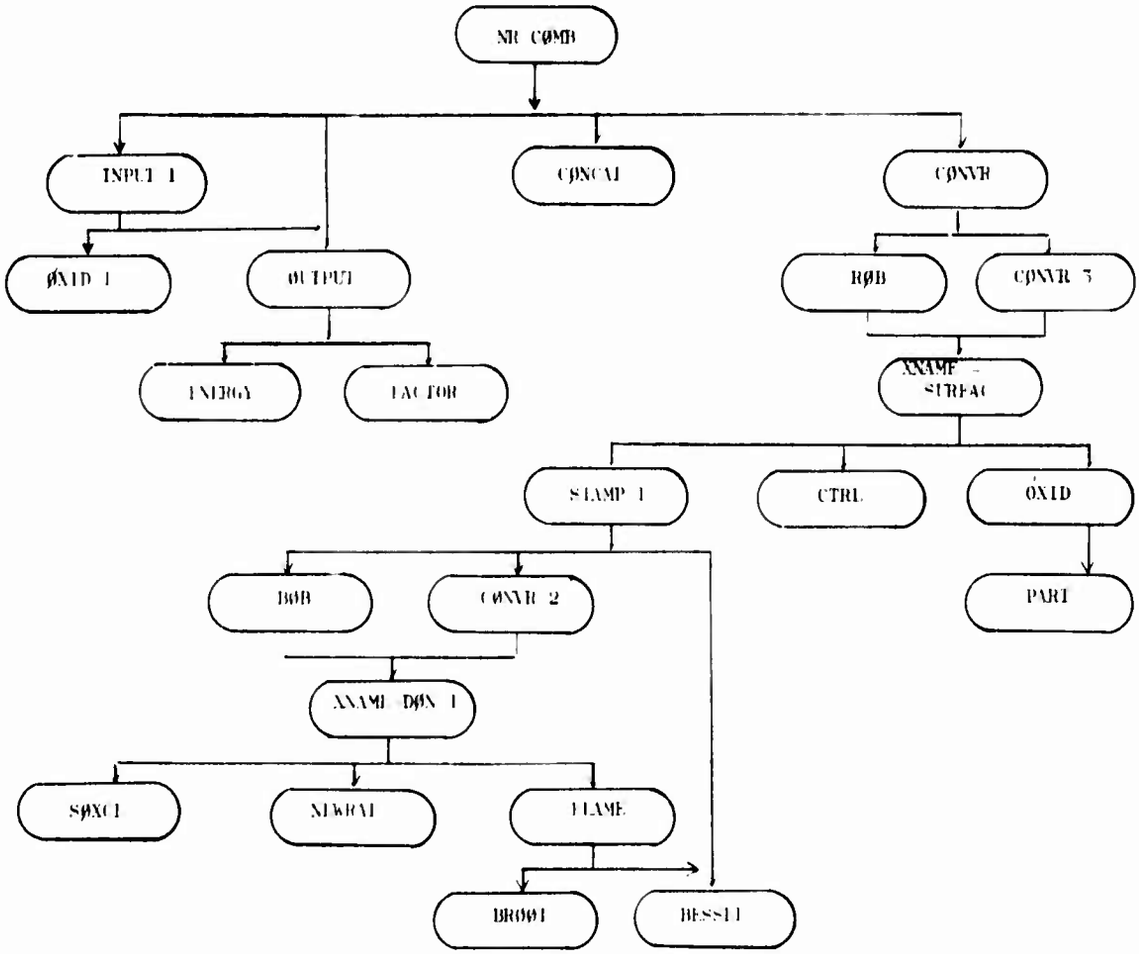
COMPUTER PROGRAM

The NRCOMB Computer Program, listed completely in Appendix B, is written in FORTRAN IV. It has been checked out on an IBM 360 and has been used to estimate the burning rate of composite solid propellants having carboxyl-terminated and hydroxyl-terminated polybutadiene binders.

A flow-chart of NRCOMB is reproduced in Figure 1.

FIGURE 1

SUBROUTINE FLOW CHART OF
COMBUSTION MODEL COMPUTER PROGRAM



NRCØMB is the main program. Its sole function is to control program flow. Calculations are carried out in the subroutines.

Subroutine INPUT does as its name implies--inputs the parameters used to calculate burning rate. These parameters are listed in detail in the section "SAMPLE PROBLEM: PROGRAM INPUTS USED TO COMPUTE BURNING RATE."

Subroutines ØUTPUT, ENERGY and FACTØR are output routines that print out parameter names and values and column heads burning rate vs. pressure data, flame parameter vs. pressure data, etc.

Subroutine CØNCAL increments the pressure from a start value to a stop value.

Function subroutines BØB and RØB establish the functional relationships XNAME = DØN 1 and XNAME = SURFAC.

Function subroutines CØNVR 2 and CØNVR 3 are convergence routines that force convergence on the desired value when upper and lower extremes are known. CØNVR 2 yields surface temperature; CØNVR 3 yields critical AP particle size.

The group of subroutines and function subroutines CØNVR, RØB, CONVR 3, CRTL, ØXID and PART utilize the multi-modal oxidizer particle size input to compute an average particle size, critical AP size, fraction of AP greater and less than critical, and an oxidizer ignition time. The roles of RØB and CØNVR 3 have been described. CRTL computes a critical AP size; ØXID computes an average diameter and a greater and less than critical size weight fraction. PART computes the AP ignition time utilizing the AP particle size distribution.

Subroutine STAMP 1, utilizing several subroutines for the competing flame, computes surface temperature and as a final

step calculates burning rate using the expression: Total Mass Flow/Propellant Density. STAMP 1 calls on BØB and CØNVR 2, both of whose roles have been described. It also calls on DØN 1 which in turn calls on SØXCAL, NEWRAF, FLAME, BESSEL and BRØØT.

Function subroutine DØN 1 computes propellant surface temperature. It uses SØXCAL to compute the fraction of total propellant surface involved in AP only decomposition. It utilizes FLAME, BESSEL, BRØØT and NEWRAF to compute the parameters needed in primary diffusion flame and final flame calculations.

SAMPLE PROBLEM: PROGRAM INPUTS USED TO COMPUTE BURNING RATE

Given here are descriptions of the program inputs used to estimate propellant burning rate. For this example, a typical low-smoke HTPB propellant having the composition listed below has been selected.

Ingredient	Weight Percent
HTPB Binder	12.0
Ammonium Perchlorate	
400 μ (nominal diameter)	55.5
200 μ (nominal diameter)	13.0
80 μ (nominal diameter)	12.2
7-11 μ (finely ground)	5.0
Aluminum, 5 μ	0.3
	100.0

Oxidizer Particle Size and Weight Fractions - INPUTS DMAX, DMIN, AND SIG

The oxidizer particle size distribution given in the formulation is broken down into several particle size weight fraction ranges for inputing by using the typical AP particle size analytical data given in Table 1. Such an input for the example propellant is shown here.

DMAX(μ)	DMIN(μ)	SIG	Subscript
600	420[a]	0.205	1
420	230[b]	0.357	2
230	140[b]	0.265	3
140	72[c]	0.096	4
72	60[d]	0.027	5
60	9.8[e]	0.039	6
9.8	3[e]	0.011	7

(a) From nominal 400μ fraction
(b) From nominal 400μ and 200μ fractions
(c) From nominal 200μ and 80μ fractions
(d) From nominal 200μ, 80μ and 7-11μ fractions
(e) From nominal 80μ and 7-11μ fractions

The 600-420 fraction is obtained by multiplying 0.555 by 0.37; the 420-230 fraction by multiplying 0.555 by 0.59 and 0.13 by 0.23 and using the sum, etc.; to produce a 7-modal AP distribution (NN = 7) input.

TABLE I

TYPICAL AP PARTICLE SIZE DISTRIBUTIONS

A. Nominal 400 μ AP (as received)

Particle Diameter Range (Microns)	Weight Percent
600-420	37.0
420-350	29.0
350-250	30.0
250-210	1.0
210-177	1.0
177-74	2.0

B. Nominal 200 μ AP (as received)

Particle Diameter Range (Microns)	Weight Percent
500-230	23.0
230-140	59.0
140-78	13.0
78-25	5.0

C. Nominal 80 μ AP (as received)

Particle Diameter Range (Microns)	Weight Percent
110-72	60
72-54	20
54-35	10
35-11	8
11-4.3	2

D. Fine Grind - Rocketdyne's Nominal 7-11 μ AP

Particle Diameter Range (Microns)	Weight Percent
80-60	5
60-9.8	75
9.8-5	15
5-3	5

Modality of AP - Input NN

In the previous section, the oxidizer was divided into a 7-modal distribution. So this input is: NN = 7

Weight Fraction Oxidizer and Aluminum - Inputs ALFA and EPS

From the formulation, it is evident that the values are:

ALFA = .857

EPS = .003

Density of Oxidizer, Binder and Aluminum - Inputs RHØX, RHØF and RHAL

Values for these quantities are (standard values):

$RH\emptyset X = 1.95\ gm/cm^3$

$RH\emptyset F = 0.91\ gm/cm^3$

$RHAL = 2.70\ gm/cm^3$

Initial Propellant Temperature and Flame Temperature - Inputs TZERO and TF

Flame temperature value is obtained from thermodynamic calculations. Values for these inputs for the example propellant are:

TZERØ = 300 K

TF = 2908 K

Binder and Oxidizer Kinetic Parameters - Inputs AF, EF, AØX and EØX

Pyrolysis rates for the separate fuel and oxidizer components are expressed by Arrhenius expressions of the form:

$$\dot{m} = A\exp\left(E/RT_s\right)$$

where A and E are input parameters. For the fuel component, the frequency factor AF = 299 gm/cm^2 sec and activation energy EF = 16,900 cal/mole which were obtained by pyrolyzing an HTPB binder[7] are used as inputs. For the oxidizer component, ammonium perchlorate, AØX values ranging from 10^4 to 10^{20} and EØX values ranging from 17,000 to 73,400 for pure AP have been reported. For use here, we have selected frequently used values in modeling studies--namely, AØX = 4 x 10^7 gm/cm^2 sec and EØX = 30,000 cal/mole.

Gaseous Diffusivity - D_o Input as GAMMA

In this program, gaseous diffusivity is calculated using Beckstead, et al's expression[3][4].

$$D = D_o \left[\frac{T^{1.75}}{P} \right]$$

D_o is an input parameter. It is estimated using the Chapman-Enskog relation[5].

$$D_{AB} = 0.0018583 \left[\frac{\sqrt{T^3 \left(\frac{1}{M_A} + \frac{1}{M_B} \right)}}{P \, \sigma^2_{AB} \Omega_{D_{AB}}} \right]$$

and

$$D_o = D_{AB} \left(\frac{P_o}{T_o^{1.75}} \right) = D_{AB} \left[\frac{1}{(273.2)^{1.75}} \right]$$

For this sample calculation, we have assumed that the gaseous fuel species is C_3H_8 which is consistent with the PMW value given in a later section. For oxidizer we have used O_2. Using appropriate values for these gases in the Chapman-Enskog equation, a value for C_3H_8-O_2 diffusion of 0.0928 cm^2/sec is obtained which yields the value of D_o below.

$$D_o = 5.07 \times 10^{-6} \text{ (input as GAMMA) } cm^2/sec$$

D_{AB} might also be estimated using the empirical relationship developed by Gilliland which can be found in many chemical engineering textbooks[6].

Ammonium Perchlorate Oxidizer
Flame Temperature - Input TAP

This is the temperature of one of the three competing flames--the temperature of the oxidizer monopropellant flame. The standard value used by Beckstead[3][4] is used here.

$$TAP = 1400 \text{ K}$$

Stoichiometric Ratios of the Primary Flame
and of the Final Flame - Inputs XNUP and XNU1

To estimate these stoichiometric ratios, the general formula below is used:

$$\text{(Stoichiometric Ratio)} = \frac{\text{Moles Fuel Species/Gram}}{\text{Moles Oxygen/117.5}}$$

AP decomposition can be represented by the stoichiometric equation:

$$NH_4ClO_4 \longrightarrow 0.5\ N_2 + 0.8\ HCl + 1.6\ H_2O + 0.5\ Cl_2 + 1.2\ O_2$$

which gives a molar oxygen flow rate of $\frac{1.2}{117.5} = 0.0102$ moles oxygen/gm

The approximate formula for an HMDI cured Poly BD R-45M HTPB binder (the formula used for material balance in thermodynamic calculations) provides a basis for estimating the moles of fuel per gram of fuel flow. Using this formula and setting the heaviest species at C_7 gives the following:

$$C_{21.15}H_{31.95}O_{.753}N_{.258}(\text{mole w/}\approx 300)^* \longrightarrow \begin{cases} 3\ C_7 \text{ Species} \\ \text{or} \\ 7\ C_3 \text{ Species} \\ \text{or} \\ 16\ CH_2 \text{ Species} \end{cases}$$

--about 8.7 moles of fuel species per 300 grams of binder on the average so that

$$XNUP = \frac{8.7/300}{0.01} = 2.9$$

---

* Polybutadiene is $\{CH_{1.5}\}_X$

In the final diffusion flame further breakdown of the binder decomposition products is assumed so that

$$C_{21.15}H_{31.95}O_{.753}N_{.258} \xrightarrow{\text{or}} \begin{cases} 7 \ C_3 \text{ Species} \\ 16 \ CH_2 \text{ Species} \end{cases}$$

This is, on the average, 11.5 moles of fuel species. This gives

$$XNU1 = \frac{11.5/300}{0.01} = 3.83$$

The diffusion flame solution employed in this model requires XNUP and XNU1 values greater than 2.8.

Molucular Weights for the Primary and Final Flames - Inputs PMW and GMW

To be consistent with stoichiometric ratios these values are calculated as follows:

$$\text{Mole Wt.} = \frac{(300 + 117)}{(\text{Moles Fuel} + \text{Moles } O_2)}$$

giving

$$PMW = \frac{417}{9.9} \approx 42$$

$$GMW = \frac{417}{12.7} \approx 33$$ (Average mole wt. of combustion products of this propellant is approx. 30)

Burning Surface Temperature--Input TS

The program calculates the temperature of the burning surface. This calculation requires an initial estimate. For use in this example:

$$TS = 750 \text{ K}$$

Flame Height Factor and Oxidizer Ignition Delay Time Parameters--Inputs AFH, CIGN, PØWIGN, and PØWD

AFH = 0.5

CIGN = 190 sec atm^m/cm^n

PØWIGN = 0.75 (an exponent: m)

PØWD = 0.8 (an exponent: n)

The flame height factor and ignition delay time parameters are those used by both Hermance and Beckstead[1][2][3][4].

Rate Constant Parameters for the Diffusion and AP Flames--Inputs KPF, KAP1 and KAP2

These are the rate constants for gas phase reactions of arbitrary reaction order and expressed in the following general form

$$\omega = k P^{\sigma}$$

Values used here for these k's are

KPF = 30 gm/cm^3 sec Atm

KAP1 = 1.12 gm/cm^3 sec Atm

KAP2 = 2.13 gm/cm^3 sec Atm

These are "standard" values for the gas phase rate constants.

Reaction Order Constants for Diffusion Flame and AP Flame--Inputs XN1, XN2, and XN3

XN1 = 1.5

XN2 = 1.8

XN3 = 1.8

These values should be considered "standard" values for the σ parameters in AP composite propellants.

Average C_p Value for Flames and Solids and Gas Conductivity - Inputs CSUBP and XLAMB

C_p is used in this model in several calculations. For example:

(1) The energy balance term accounting for propellant heat up

$$m_t C_p (T_s - T_o)$$

(2) As an enthalpy term in the AP flame relationship

$$C_p (T_{AP} - T_o)$$

(3) In non-dimensional standoff distance calculations in the multipliers

$$\frac{C_p M_t}{\lambda} \text{ and } \frac{C_p M_{ox}}{\lambda}$$

Each requires a C_p value. This model, like the BDP model uses only one C_p value for both gases and solids. This value is an overall average value. Why this approximate approach has been used becomes evident on calculating this overall average value.

The specific heat of AP below and above the phase transition temperature yields an average value

$$C_p = \frac{.309 + .365}{2} = 0.337 \text{ cal./gm-K}$$

The specific heat of the example propellant is

$$C_p = 0.352 \text{ cal/gm-K}$$

Each gaseous product contributes its proportional share to C_p. To obtain the C_p value for the AP flame, the products shown in the stoichiometry section provided the basis for the material balance and the AP flame temperature and propellant surface temperature provided the average temperature from which the C_p contributions in the table were obtained.

$$T(ave) = \frac{750 + 1400}{2} = 1075 \text{ K}$$

Gas	Wt. Fraction	C_p Contribution*
N_2	0.096	0.0259
HCl	0.201	0.0386
H_2O	0.198	0.1026
Cl_2	0.241	0.0300
O_2	0.264	0.066

* Estimated from charts in Hougen and Watson, "Chemical Process Principles: Part One - Material and Energy Balances," John Wiley

These contributions sum up to the C_p value for the AP flame.

$$C_p = 0.263 \text{ cal/gm - K}$$

To obtain the C_p value for the propellant flame, the final combustion product distribution was used to provide an estimated average value at an average temperature as shown below:

$$T(\text{ave.}) = \frac{\text{Surface Temp + Flame Temp.}}{2} = \frac{750 + 2910}{2} = 1830 \text{ K}$$

Gas	Wt. Fraction*	C_p Contribution**
N_2	0.102	0.0287
H_2O	0.286	0.1604
CO_2	0.173	0.0500
CO	0.174	0.0491
HCl	0.265	0.0560

* From flame temperature calculations

** Estimated from charts in Hougen and Watson, "Chemical Process Principles: Part One - Material and Energy Balances," John Wiley.

These tabulated contributions sum up to

$$C_p = 0.344 \text{ cal/gm - K}$$

In arriving at these C_p values for the flames, ideal gas behavior has been assumed.

The overall average of these values is used as input.

$$CSUBP = \frac{0.337 + 0.352 + 0.263 + 0.344}{4} = 0.324 \text{ cal/gm - K}$$

Beckstead's "Standard" value[3][4] for gas conductivity (ideal behavior assumed) is used here as gas conductivity input.

$$XLAMB = 0.0003 \text{ cal/cm sec - K}$$

Aluminum Heat Absorption - Input QAL

The latent heat of fusion - the heat absorbed when molten drops of aluminum are formed on the propellant surface--is input.

$$QAL = \left[\text{(Heat of Fusion)} + \left\langle C_p \text{ (mean) x 660}\right\rangle\right] = 257 \text{ cal/gm}$$

Heat to Vaporize the Fuel Binder - Input QFUEL

For this input the measured value for an HTPB binder[7] is used.

$$QFUEL = 433 \text{ cal/gm}$$

Heat Stemming from AP Decomposition, Reaction of Less Than Critical Size AP with Fuel, and from Liquid Layer--Inputs QL, QSOLID and QLIQ

The BDP model employed a QL input only to account for decomposition of the oxidizer, AP, at the surface[3][4]. This parameter, QL, was varied to account for more or less reaction in the solid phase. Mr. Sammons introduced two additional adjustable parameters,

QSOLID and QLIQ, to account for reaction in the solid phase. Here the following values for these parameters (values used by Sammons) are input.

QL = 0.0 cal/gm
QSØLID = 1085.0 cal/gm
QLIQ = 1000.0 cal/gm

Pressure Programming Inputs PSTART and PSTØP

Two pressure programming inputs to start and stop the incremental pressure increases employed in calculating a burning rate vs. pressure curve are required. Inputs used here are:

PSTART = 1.0
PSTØP = 220.0

Pressures used in the burning rate calculations are in atmospheres. These pressures are converted to psia before outputing.

SAMPLE PROGRAM RUN

Following are the computer inputs and computer printout obtained with the example data described in the previous section.

CARD 1: TITIE CARD

NO. REQUIRED: One card per run

FUNCTION: Identify run output

FORMAT: (20A4)

Column	Format	Variable	Description
2--80	20A4	TIT1	79 columns of alphanumeric data may be input to identify run

CARD 2: CONTROL CARD

NO. REQUIRED: One card per run

FUNCTION: Specify run options to be executed

FORMAT: (12I6)

Column	Format	Variable	Description
1--6	I6	NJØB	Specifies run option 1 - Input complete set of data (NJØB must always be 1 for first run) 2 - Stacked run; input new values for AF and AØX 3 - Stacked run; input new value for QL 4 - Stacked run; input new value for XNU1 5 - Stacked run; input new value for AFH 6 - Stacked run; input new values for PSTART and PSTOP 7 - Stacked run; input new values for IX and TZEKO 8 - Stacked run; input new value for QF 9 - Stacked run; input new modality of oxidizer and aluminum weight fraction 10 - Rerun same problem - not used 11 - Rerun using weight fraction and modality of oxidizer data stored in INPUT1 100 - Repeat printout of last run 105 - Repeat last run - printout only HDN1, HDP1 and SØX1
7--12	I6	IPLØT	If IPLØT > 0, do not print propellant data input
13--18	I6	IPLT	0--Do not write tape for plotting 2--Write log(P) and log (rate) on logical unit 10 for plotting. Do not print output. ≠0, ≠2 --Write log (P) and log (rate) on logical unit 10 for plotting and print output
19--80	--	--	Not read - may be used to identify card

CARD 3: DATA CARD

NO. REQUIRED: One card per run for NJOB=1

FUNCTION: Specify propellant parameters

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	TZERO	Initial propellant temperature, deg K
13--24	E12.5	ALFA	Oxidizer weight fraction
25--36	E12.5	TF	Flame temperature, deg K
37--48	E12.5	GMW	Molecular weight of final flame
49--60	E12.5	XNU1	Stoichiometric ratio of the final flame > 2.8
61--72	E12.5	DZERO	Mean AP particle size, μ input as 0.0 for multimodal AP
73--80	--	--	Not read - may be used to identify card

CARD 3A: DATA CARD

NO. REQUIRED: One card per run for NJOB=2 through 8
(Do not include for NJOB=1 or NJOB > 8)

FUNCTION: Specify input data changes to previous run

FORMAT: As noted

Column	Format	Variable	Description	
1--12	E12.5	AF	Frequency factor--See Card 4	NJOB=2
13--24	E12.5	AØX	Frequency factor--See Card 5	
1--12	E12.5	QL	Heat from AP decomposition, cal/gm	NJOB=3
1--12	E12.5	XNU1	Stoichiometric ratio of final flame > 2.8	NJOB=4
1--12	E12.5	AFH	Flame height factor	NJOB=5
1--12	E12.5	PSTART	Pressure to start incremental calculations, atm	NJOB=6
13--24	E12.5	PSTOP	Pressure to stop incremental calculations, atm	
1--6	I6	IX	Output control(1)	NJOB=7
7--12	6X	--	Blank	
13--24	E12.5	TZERO	Initial propellant temperature, deg K	
1--12	E12.5	QFUEL	Heat to vaporize the fuel binder, cal/gm	NJOB=8

(1)

IX = 1 Normal output
2 Print energy terms vs pressure in subroutine energy
3 Print weight factors with respect to critical particle size and critical particle size vs pressure in subroutine factor
4 Print burning rate and XTAR's vs pressure only

CARD 4: DATA CARD

NO. REQUIRED: One card per run for NJOB=1

FUNCTION: Specify propellant parameters

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	QFUEL	Heat to vaporize the fuel binder, cal/gm
13--24	E12.5	RHOF	Density of binder, gm/cm^3
25--36	E12.5	AF	Frequency factor,[1] gm/cm^2-sec
37--48	E12.5	EF	Activation energy,[1] cal/mole
49--60	E12.5	XNUP	Stoichiometric ratio of the final flame > 2.8
61--72	E12.5	PMW	Molecular weight of primary flame
73--80	--	--	Not read - may be used to identify card

[1] Kinetic parameters used to calculate binder pyrolysis rates were:

$$\dot{m} = AF \exp(EF/RTs)$$

CARD 5: DATA CARD

NO. REQUIRED: One card per run for NJOB=1

FUNCTION: Specify propellant parameters

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	QL	Heat from AP decomposition, cal/gm
13--24	E12.5	RHOX	Density of oxidizer, gm/cm^3
25--36	E12.5	AOX	Frequency factor(1), gm/cm^2-sec
37--48	E12.5	EOX	Activation energy(1), cal/mole
49--60	E12.5	TAP	Ammonium perchlorate flame temperature, deg K
61--72	E12.5	--	Not used
73--80	--	--	Not read - may be used to identify card

(1) Kinetic parameters used to calculate oxidizer pyrolysis rates were:

$$\dot{m} = AOX \exp(EOX/RTs)$$

CARD 6: DATA CARD

NO. REQUIRED: One care per run for NJOB=1

FUNCTION: Specify oxidizer ignition parameters and pressure range for calculations

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	CIGN	Oxidizer ignition delay time coefficient(1), sec-atm^{POWIGN}/cm^{POWD}
13--24	E12.5	POWIGN	Oxidizer ignition delay time pressure exponent(1)
25--36	E12.5	POWD	Oxidizer ignition delay time diameter exponent(1)
37--48	E12.5	PSTART	Pressure to start incremental calculations, atm
49--60	E12.5	PSTOP	Pressure to stop incremental calculations, atm
61--72	E12.5	--	Not used
73--80	--	--	Not read - may be used to identify card

(1) Oxidizer ignition delay time parameters use in the following expression:

$$\frac{n}{Do} = \frac{1}{2}\left(1 \pm \frac{1}{\sqrt{3}}\right)\left(1 - \frac{r_{ox}}{r_f}\right) + r_{ox}\,\frac{CIGN*Do^{POWD}}{p^{POWIGN}}$$

CARD 7: DATA CARD

NO. REQUIRED: One card per run for NJOB=1

FUNCTION: Specify rate and reaction order constants for diffusion flame and AP flame

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	KPF	Rate coefficient for diffusion flame, gm/cm^3-sec-atm
13--24	E12.5	KAP1	Rate coefficient #1 for AP flame, gm/cm^3-sec-atm
25--36	E12.5	KAP2	Rate coefficient #2 for AP flame, gm/cm^3-sec-atm
37--48	E12.5	XN1	Reaction order constant for diffusion flame
49--60	E12.5	XN2	Reaction order constant #1 for AP flame
61--72	E12.5	XN3	Reaction order constant #2 for AP flame
73--80	--	--	Not read - may be used to identify card

CARD 8: DATA CARD

NO. REQUIRED: One card per run for NJOB=1

FUNCTION: Specify thermal properties and flame height

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	CSUBP	Specific heat of flame, cal/gm-deg K
13--24	E12.5	XLAMB	Gas conductivity, cal/cm-sec-deg K
25--36	E12.5	GAMMA	Gaseous diffusivity, cm^2/sec
37--48	E12.5	AFH	Flame height factor
49--60	E12.5	--	Not used
61--72	E12.5	--	Not used
73--80	--	--	Not read - may be used to identify card

CARD 9: DATA CARD

NO. REQUIRED: One card per run NJOB=1

FUNCTION: Specify propellant parameters

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	TS	Initial estimate of burning surface temperature, deg K
13--24	E12.5	QSØLID	Heat from reaction of less than critical size AP with fuel, cal/gm
25--36	E12.5	QLIQ	Heat from liquid layer, cal/gm
37--48	E12.5	QAL	Aluminum heat absorption, cal/gm
49--60	E12.5	RHAL	Density of aluminum, gm/cm^3
61--72	E12.5	--	Not used
73--80	--	--	Not read - may be used to identify card

CARD 10: DATA CARD

NO. REQUIRED: One card per run for NJOB=1 or NJOB=9

FUNCTION: Specify modality of AP particle size distribution

FORMAT: (12I6)

Column	Format	Variable	Description
1--6	I6	NN	Modality of AP particle size distribution
7--72	11I6	--	Not used
73--80	--	--	Not read - may be used to identify card

CARD 11: DATA CARD

NO. REQUIRED: One card for each two particle distribution modes input for NJOB=1 or NJOB=9

FUNCTION: Describe AP particle size distribution

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	SIG(1)	Weight fraction of AP particles between DMIN(1) and DMAX(1)
13--24	E12.5	DMIN(1)	Minimum diameter of particles in this mode, microns
25--36	E12.5	DMAX(1)	Maximum diameter of particles in this mode, microns
37--48	E12.5	SIG(2)	Weight fraction of AP particles between DMIN(2) and DMAX(2)
49--60	E12.5	DMIN(2)	Minimum diameter of particles in this mode, microns
61--72	E12.5	DMAX(2)	Maximum diameter of particles in this mode, microns
73--80	--	--	Not read - may be used to identify card

CARD 12: DATA CARD

NO. REQUIRED: One card per run for NJOB=1 or NJOB=9

FUNCTION: Specify weight fraction aluminum

FORMAT: (6E12.5)

Column	Format	Variable	Description
1--12	E12.5	EPS	Weight fraction of aluminum
13--72	E12.5	--	Not used
73--80	--	--	Not read - may be used to identify card

CARD 13: DATA CARD

NO. REQUIRED: One card per run except for NJOB=105

FUNCTION: Specify print option

FORMAT: A4

Column	Format	Variable	Description
1--4	A4	LAN	Specifies printout option--YES blank in columns 1--4 implies printout only rate vs pressure. Any other entry will cause printout to include surface temperature, CRIT, n/Do, MØX, SØX, and XTAR vs pressure to be printed.

CARD 14: TITLE CARD

NO. REQUIRED: One card per run

FUNCTION: Specify end of job or title of next run

FORMAT: (20A4)

Column	Format	Variable	Description
1--80	20A4	TIT1	79 columns (2--80) of alphanumeric data may be input to identify stacked run. END OF JOB in columns 1--10 implies end of job and computer will terminate normally.

NOTE: If stacked job is to be run, repeat input indicated for Cards 2 through 13 as required by NJOB value specified in Card 2.

RESULTS OBTAINED WITH EXAMPLE DATA

BURNING RATES - 7 MODAL AP - 86% SOLIDS - 0.3% ALUMINUM

PROPELLANT DATA IS

WT PERCENT OXID = 85.7	MEAN DIAM OF 273.8 MICRON
DELDI = 0.0749	PROP DENSITY = 1.68
BINDER DENSITY = 0.91	OXID DENSITY= 1.95
QFUEL = 433.0	TF(DEG K) = 2908.
MOL WT = 33.00	PRI MOL WT = 42.00
DIFF PARAM = 0.5070E-05	BESS FUNCT = 0.1339
ST RAT = 2.83	PRI ST RAT = 2.90

OXIDIZER IGNITION AND BURNING DATA IS

CIGN = 190.0	POWIGN = 0.750
POWD = 0.8	LATENT HEAT = 0.0

ACTIVATION ENERGIES AND RATE FACTORS ARE

EF = 16800.	E OX = 30000.
AF = 0.299E+03	A OX = 0.400E+08
ORDER,PF = 1.500	RT CON, PF = 0.300E+02
ORDER,LP = 1.800	RT CON, LP = 0.112E+01
ORDER,HP = 1.800	RT CON, HP = 0.213E+01

FLAME PROPERTIES ARE

OXID FLM TEMP = 1400.0	GAS CONDUCT = 0.00030
CP(AVE) = 0.3240	QFF = 700.9
QPF = 906.0	AV FLM HT FACT = 0.5000

PROPELLANT INITIAL TEMP IS 27.0 DEG CENTIGRADE

PT ATMS	PT, PSIA	BR, CM/SEC	BR, IN/SEC	SURF T	CFIT
6.80	100.0	0.1732	0.0682	531.07	16.440
8.16	120.0	0.1776	0.0699	532.14	15.228
10.20	150.0	0.2007	0.0790	537.49	14.771
13.61	200.0	0.2466	0.0971	546.64	12.563
17.01	250.0	0.2928	0.1153	554.42	10.978
20.41	300.0	0.3375	0.1329	560.97	9.841
27.21	400.0	0.4309	0.1697	572.43	8.068
34.01	500.0	0.5049	0.1988	580.04	7.093
47.62	700.0	0.6357	0.2503	591.34	5.972
68.03	1000.0	0.7926	0.3120	602.44	4.889
81.63	1200.0	0.8779	0.3456	607.68	4.487
102.04	1500.0	0.9854	0.3880	613.69	4.072
136.05	2000.0	1.1287	0.4444	620.85	3.631
170.07	2500.0	1.2445	0.4899	626.07	3.341
204.08	3000.0	1.3430	0.5287	630.19	3.126
272.11	4000.0	1.5156	0.5967	636.78	2.819

PT ATM	HDP	HDN	MOX	SOX
6.80	-0.5000	-0.5000	0.2813	0.8679
8.16	-0.5000	-0.5000	0.2885	0.8680
10.20	-0.5000	-0.5000	0.3265	0.8688
13.61	-0.5000	-0.5000	0.4019	0.8703
17.01	-0.5000	-0.5000	0.4779	0.8715
20.41	-0.5000	-0.5000	0.5514	0.8725
27.21	-0.5000	-0.5000	0.7048	0.8733
34.01	-0.5000	-0.5000	0.8263	0.8738
47.62	-0.5000	-0.5000	1.0414	0.8746
68.03	-0.5000	-0.5000	1.2996	0.8753
81.63	-0.5000	-0.5000	1.4400	0.8756
102.04	-0.5000	-0.5000	1.6172	0.8760
136.05	-0.5000	-0.5000	1.8534	0.8764
170.07	-0.5000	-0.5000	2.0443	0.8768
204.08	-0.5000	-0.5000	2.2069	0.8770
272.11	-0.5000	-0.5000	2.4910	0.8772

PT, PSIA	BP, IN/SEC	XTAR PD	XTAR PF	XTAR AP	XTAR D
100.0	0.0682	40.27	5.47	79.65	2.57
120.0	0.0699	40.94	4.27	58.82	2.60
150.0	0.0790	44.10	3.45	44.55	2.73
200.0	0.0971	50.31	2.76	32.67	2.98
250.0	0.1153	56.47	2.34	26.00	3.25
300.0	0.1329	62.32	2.05	21.61	3.51
400.0	0.1697	27.54	1.70	16.46	4.23
500.0	0.1988	31.12	1.43	12.91	4.78
700.0	0.2503	37.26	1.08	8.88	5.76
1000.0	0.3120	44.34	0.79	5.83	6.93
1200.0	0.3456	48.07	0.67	4.65	7.55
1500.0	0.3880	52.67	0.54	3.50	8.34
2000.0	0.4444	58.64	0.40	2.39	9.37
2500.0	0.4899	63.33	0.31	1.76	10.19
3000.0	0.5287	67.24	0.26	1.37	10.89
4000.0	0.5967	74.83	0.19	0.92	12.20

Combustion modeling studies will be continued during FY 1975. These further studies will be directed primarily toward addition of a mathematical treatment for heterogeneous catalysis of burning rate to the multiple-flame model.

REFERENCES

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(3) Lockheed Propulsion Company, "Combustion Tailoring Criteria for Solid Propellants," Final Report, AFRPL-TR-69-190, May 1969.

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(5) Bird, R. B., W. E. Stewart and E. N. Lightfoot, "Transport Phenomena," John Wiley and Sons, Inc. (1960).

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APPENDIX I

EM 72-09 ADVANCEMENT OF COMPREHENSIVE COMBUSTION MODELING

EM 73-05 SOLID PROPELLANT COMBUSTION MODELING

FM 72-09

ADVANCEMENT OF COMPREHENSIVE COMBUSTION MODELING

By

G. D. Sammons

Presented to the JANNAF Interagency Propulsion Committee
9th JANNAF Combustion Meeting, held 11--15 September
1972 at U.S. Naval Postgraduate School, Monterey, California

ROCKETDYNE
North American Rockwell Corporation
Solid Rocket Division
McGregor, Texas

3 October 1972

I-1/R-4827

ADVANCEMENT OF COMPREHENSIVE COMBUSTION MODELING

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INTRODUCTION

Studies in many laboratories over the past 15 years on the mechanism of combustion of composite solid propellants have provided enough information that it has been possible recently to approach the goal of a truly comprehensive and practical mathematical combustion model. This paper is a progress report covering the first five months of effort under AFOSR Contract F44620-72-C-0046 with this goal as its aim.

After the pioneering effort of Prof. C. E. Hermance,[1] Beckstead, Derr and Price[2] advanced this type of modeling by introduction of their multiple-flame model. The purpose of the current work is to advance another step forward in comprehensive modeling.

In both of the earlier models, researchers found that a relatively large amount of condensed phase or surface reaction was necessary. This is entirely consistent with a large volume of experimental evidence gathered in recent years.[3,4,5,6] A concept of critical particle size for ammonium perchlorate (AP) was presented recently[3] that allows the actual calculation of condensed phase heat release. This theory is based on the concept that a critical particle size exists for AP such that all particles beneath this size are consumed in condensed phase reaction.

MATHEMATICAL TECHNIQUE

The critical particle size is arrived at by calculating at a specific pressure the thermal wave penetration into the solid phase sufficient to cause a very fast condensed phase reaction. Initially in this study, a simple limiting thermal gradient was calculated by dividing the burn rate by the propellant thermal diffusivity and multiplying by the difference between surface temperature and a temperature at which the rate of condensed phase reaction becomes rapid enough to occur in the residence time available.

Figure 1 shows the surface energy balance incorporating the critical particle size model. The symbols M_{ox} and S_{ox} are defined as the mass flux and burning surface of supercritical oxidizer. M_p is the mass flux of fuel binder plus subcritical oxidizer. Delta is the weight fraction of this interstitial propellant that is consumed in condensed phase reaction and is calculated based on stoichiometry considerations.

The flame heights are calculated by the Burke-Schuman treatment as modified for short flames by Beckstead.[2] A planned improvement in this calculation is to use more terms of the series solution. Use of the first term gives only a rough approximation.[7]

Equations actually used in the computer program are presented in

Fig. 2. The first is an equation for surface temperature that is derived from the surface energy balance using mass balance equations. The coefficient gamma is the weight fraction of supercritical oxidizer in the propellant. The computer program iterates on surface temperature with an estimated value of critical particle size and after convergence a critical size is calculated. The surface temperature is then recalculated if the initial and calculated critical particle sizes are different. This doubly iterative process is continued until convergence of critical particle size is obtained within 0.01 micrometers. The equations for the unit heat release in the primary and final flame are also shown in Fig. 2. They also include the calculation of condensed phase heat release and the coefficient delta.

ENERGY TO RAISE PROPELLANT TO T_s | ENERGY TO VAPORIZE OXIDIZER | ENERGY TO VAPORIZE FUEL | ENERGY FROM CONDENSED PHASE

$$m_t c_p (T_s - T_o) = - m_{ox} \frac{S_{ox}}{S_o} Q_L - (1-\delta) m_p \frac{S_p}{S_o} Q_f + \delta m_p \frac{S_p}{S} Q_s$$

ENERGY FROM PRIMARY DIFFUSION FLAME | ENERGY FROM AP FLAME | ENERGY FROM FINAL DIFFUSION FLAME

$$+ \beta_F Q_{PF} m_t \exp\left(-\dot{\xi}_{PF}\right) + (1-\beta_F) m_{ox} \frac{S_{ox}}{S_o} \left[Q_{AP} \exp\left(\dot{\xi}_{AP}\right) + Q_{FF} \exp\left(\dot{\xi}_T\right)\right]$$

Figure 1. Critical Particle Size Model Energy Balance

SURFACE TEMPERATURE

$$T_s = T_o - \frac{\gamma}{C_p} Q_L - \frac{(1-\delta)(1-\gamma)}{C_p} Q_f + \frac{\delta(1-\gamma)}{C_p} Q_s + \frac{\beta_F Q_{PF}}{C_p} \exp\left(-\dot{\xi}_{PF}\right) + (1-\beta_F) \frac{\gamma}{C_p} \left[Q_{AP} \exp\left(-\dot{\xi}_{AP}\right) + Q_{FF} \exp\left(-\dot{\xi}_T\right)\right]$$

PRIMARY FLAME

$$Q_{PF} = C_p (T_f - T_o) + \gamma Q_L + (1-\delta)(1-\gamma) Q_f - \delta(1-\gamma) Q_s$$

FINAL FLAME

$$Q_{FF} = \frac{C_p}{\gamma} \left[(T_f - T_o) - \gamma (T_{AP} - T_o)\right] + \frac{(1-\delta)(1-\gamma)}{\gamma} Q_f - \frac{\delta(1-\gamma)}{\gamma} Q_s$$

Figure 2. Equations Used in Computer Program

COMPUTER PROGRAM

There are several reasons that a time share computer was used for this work. One is speed of turnover; for instance, 15 or 20 turnovers are obtained within 30 minutes as opposed to one or two a day with conventional hardware. It allows direct communication with a large, fast computer and the editing software is extremely versatile. Additionally, it provides a way for an engineer not versed in computer technology to easily run a complex program with varying inputs. It is hoped that this program will eventually be a tool for engineers and chemists.

Figure 3 shows two types of input that are most commonly used. There are many other optional inputs what can be used if desired. The input on the left uses a data file called FLEXI to input about 30 ingredient parameters. For this option a description of oxidizer must be typed in, which includes modality and weight fraction and minimum and maximum particle size for each mode. At this point either output can be asked for or any single parameter can be changed; for instance, in this example the unit heat

release in the condensed phase was changed. Only the information after each question mark is typed, as input all the rest is output by the computer.

```
RUN

NRCOMB    14:53  NR T/S  JULY 21, 1972

NJOB,IPLOT,IPLT
 ? 1,0,0

TITLE LENGTH, IDENTIFY THE RUN
 ? 02TEST

IS DATA FILE TO BE USED  ? YES

FILE NAME ? FLEX1

MODALITY OF OXIDIZER  ? 5

SIG(J),DMIN(J),DMAX(J)
 ? .21,230,450,
 ? .35,150,210,
 ? .12,75,142,
 ? .25-6,15.4,62.2,
 ? .06,3.8,8.9

NJOB,IPLOT,IPLT
 ? 4,0,0

QSOLID=   ? 750

NJOB,IPLOT,IPLT
 ? 10,1,0
```

```
NRCOMB    08:47  NR T/S  AUG. 09, 1972

NJOB,IPLOT,IPLT
 ? 11,1,0

FILE NAME ? FLEX1

NJOB,IPLOT,IPLT
 ? 10,1,0
```

Figure 3. Computer Printout of Theoretical Data for CTPB Propellant

The input on the right of Fig. 3 is a minimum input where all data are entered by the computer. Again, if any one parameter change is desired it can be input as was done with QSOLID in the other input. This is the input that is used for the study of parametric variations.

The simplest form of output is shown in Fig. 4. Only burn rate pressure and critical particle size are given. Particle size is in micrometers. If no subcritical AP is calculated, the critical particle size column does not appear. Additional data can be obtained without any recalculations simply by inputting the proper index. Some of the tables of parameters are shown in Fig. 5 through 8. Figure 5 lists the coefficients used in the surface temperature and other equations shown in Fig. 2. The parameters SIGC and SIGSC are the weight fractions of subcritical and supercritical AP, respectively. The

```
RATES ONLY   ? YES

 PT, PSIA     BR IN/SEC     CRIT

   100.0        0.1799     10.000
   120.0        0.1929      9.635
   150.0        0.2081      9.208
   200.0        0.2347      8.789
   250.0        0.2353      8.522
   300.0        0.2369      8.522
   400.0        0.2521      8.168
   500.0        0.2603      7.948
   700.0        0.2832      7.395
  1000.0        0.3336      6.465
  1200.0        0.3710      5.955
  1500.0        0.4289      5.280
  2000.0        0.5246      4.457
  2500.0        0.6171      3.887
  3000.0        0.7066      3.470
  4000.0        0.8685      2.899
NJOB,IPLOT,IPLT
 ? 7,0,0

IX=    ? 3

NJOB,IPLOT,IPLT
 ? 100,0,0
```

Figure 4. Continuation of Printout

sum of these is always one. Figure 6 and 7 show the calculated contributions to surface temperature in degrees Kelvin. The oxidizer and fuel vaporization are negative contributions. Figure 8 gives the flame heights in micrometers. The computer time of 30.5 seconds shown in this figure is the total time for about twice the output given in Fig. 5 through 8.

```
PT, PSIA  BR, IN/SEC  BETAP      DELTA   SIGC   SIGSC  GAMMA     CRIT

  100.0     0.1799   1.0000     0.266   0.060  0.940  0.790     10.000
  120.0     0.1929   1.0000     0.261   0.058  0.942  0.791      9.635
  150.0     0.2081   1.0000     0.252   0.056  0.944  0.793      9.208
  200.0     0.2247   1.0000     0.243   0.053  0.947  0.795      8.789
  250.0     0.2353   1.0000     0.236   0.052  0.948  0.797      8.522
  300.0     0.2369   0.8090     0.236   0.052  0.948  0.797      8.522
  400.0     0.2521   0.5028     0.228   0.049  0.951  0.799      8.168
  500.0     0.2603   0.3444     0.222   0.048  0.952  0.800      7.948
  700.0     0.2832   0.2007     0.207   0.044  0.956  0.803      7.395
 1000.0     0.3336   0.1209     0.176   0.036  0.964  0.810      6.465
 1200.0     0.3710   0.0952     0.157   0.031  0.969  0.814      5.955
 1500.0     0.4289   0.0734     0.127   0.025  0.975  0.819      5.280
 2000.0     0.5246   0.0548     0.081   0.015  0.985  0.827      4.457
 2500.0     0.6171   0.0456     0.041   0.007  0.993  0.834      3.887
 3000.0     0.7066   0.0407     0.005   0.001  0.999  0.839      3.470
 4000.0     0.8685   0.0247     0.000   0.000  1.000  0.840      2.899
NJOB, IPLOT, IPLT
 ? 7,0,0

IX=     ? 2

NJOB, IPLOT, IPLT
 ? 100,0,0
```

Figure 5. Continuation of Printout

PT, PSIA	BR, IN/SEC	OXID VAP	FUEL VAP	CP HEAT	CRIT
100.0	0.1799	0.0	0.2	104.9	10.000
120.0	0.1929	0.0	0.2	102.2	9.635
150.0	0.2081	0.0	0.2	97.8	9.208
200.0	0.2247	0.0	0.2	93.2	8.789
250.0	0.2353	0.0	0.2	90.1	8.522
300.0	0.2369	0.0	0.2	90.1	8.522
400.0	0.2521	0.0	0.2	85.9	8.168
500.0	0.2603	0.0	0.2	83.3	7.948
700.0	0.2832	0.0	0.2	76.1	7.395
1000.0	0.3336	0.0	0.2	62.9	6.465
1200.0	0.3710	0.0	0.2	54.8	5.955
1500.0	0.4289	0.0	0.2	42.9	5.280
2000.0	0.5246	0.0	0.2	26.2	4.457
2500.0	0.6171	0.0	0.2	12.7	3.887
3000.0	0.7066	0.0	0.2	1.5	3.470
4000.0	0.8685	0.0	0.2	0.0	2.899

Figure 6. Continuation of Printout

Figure 9 shows the sigmoid distribution curve usually obtained with commercial oxidizer. From this curve it is easy to see that the use of 50 percent point does not give a true representation of particle size. To improve realism in oxidizer input, a spline fit was made to the sigmoid curve and the data input as a multimodal oxidizer. The curve in Fig. 9 was input as four modes. The oxidizer handling subroutine separates the modes into supercritical and subcritical particle sizes and will divide a single mode if necessary.

```
 PI, PSIA     BR, IN/SEC    PF HEAT      APF HEAT      FF HEAT       CRIT

   100.0         0.1799       432.9          0.0          0.0       10.000
   120.0         0.1929       441.4          0.0          0.0        9.635
   150.0         0.2081       452.5          0.0          0.0        9.208
   200.0         0.2247       464.5          0.0          0.0        8.789
   250.0         0.2353       472.5          0.0          0.0        8.522
   300.0         0.2369       472.2          2.3          0.1        8.522
   400.0         0.2521       461.0         22.2          0.8        8.168
   500.0         0.2603       419.4         67.9          1.8        7.948
   700.0         0.2832       316.9        182.0          2.6        7.395
  1000.0         0.3336       218.4        305.1          1.0        6.465
  1200.0         0.3710       179.3        359.4          0.3        5.955
  1500.0         0.4289       143.4        416.4          0.1        5.280
  2000.0         0.5246       111.1        478.5          0.0        4.457
  2500.0         0.6171        94.4        519.6          0.0        3.887
  3000.0         0.7066        85.5        549.0          0.0        3.470
  4000.0         0.8685        53.1        597.9          0.0        2.899
NJOB, IPLOT, IPLT
 ? 7,0,0

IX=     ? 1

NJOB, IPLOT, IPLT
 ? 100,0,0
```

Figure 7. Continuation of Printout

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 PT, PSIA    BR, IN/SEC XTAR PD     XTAR PF     XTAR AP     XTAR D

  100.00       0.1799       11.79       14.16      205.99       25.53
  120.00       0.1929       12.41       11.54      162.44       27.22
  150.00       0.2081       13.01        8.91      120.59       29.39
  200.00       0.2247       13.76        6.25       80.57       32.12
  250.00       0.2353       14.25        4.68       58.00       34.06
  300.00       0.2369       14.59        3.59       42.93       34.82
  400.00       0.2521       15.02        2.48       27.66       37.16
  500.01       0.2603       15.11        1.83       19.18       38.29
  700.00       0.2832       15.06        1.20       11.28       40.86
  000.00       0.3336       14.86        0.83        6.82       46.27
  200.00       0.3710       14.72        0.70        5.37       50.25
  500.00       0.4289       14.26        0.58        4.07       56.47
 2000.01       0.5246       13.25        0.46        2.88       66.87
 2500.03       0.6171       12.08        0.39        2.22       77.16
 3000.01       0.7066       10.83        0.34        1.81       87.34
 4000.02       0.8685       12.40        0.27        1.29      104.33
NJOB, IPLOT, IPLT
 ? S

RUNNING TIME:   30.5 SECS   I/O TIME :   18.4 SECS

READY
BYE

OFF AT 13:50
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Figure 8. Continuation of Printout

RESULTS

The initial test of the computer program was made with the data of Bastress primarily because both Hermance and Beckstead used these data. It, therefore, provides a point of correlation between the models (Ref Fig. 10). The theoretical data from the critical particle size model are shown as points. Data for the 20-micron AP (monomodal, 70% loading) fits Bastress' data within experimental error. The fit is not as good with the 200-micron AP but it is a considerable improvement over Beckstead's last published results.[5] One of the major factors making the 200-micron monomodal propellant a better fit was to use the entire oxidizer distribution curve as input, as

was described previously. No further work is planned with this propellant, as it is not one currently in wide use. All subsequent comparisons of theoretical data will be with production or development propellants.

Figure 11 shows the theoretical data obtained for an 84% AP-loaded propellant with a carboxy-terminated polybutadiene (CTPB) binder. Experimental data shown are for an 86% AP loading. This line would swing down, pivoting at high pressure if there were only an 84% loading. The fit of data is, therefore, much better than it appears to be in Fig. 11.

All experimental data in Fig. 10 and 11 are strand rates, which are not necessarily predictive of motor rates. In the future only motor rates will be used for correlation if at all possible.

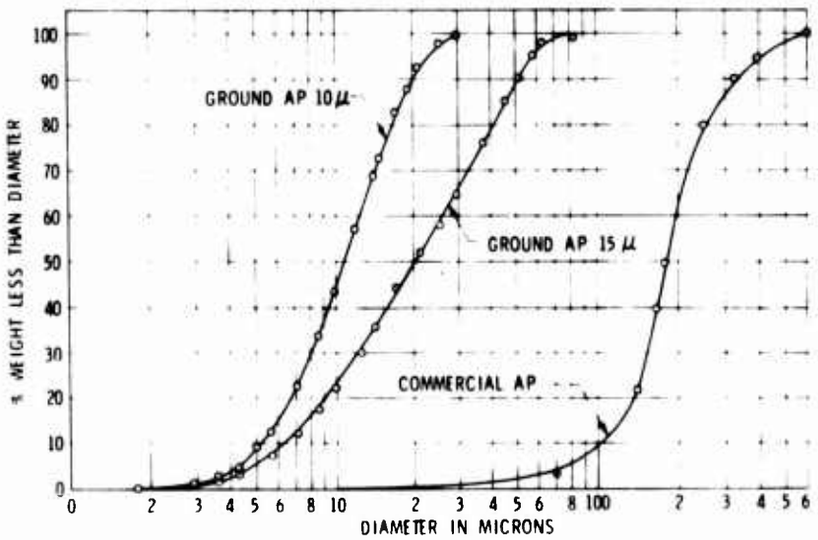

Figure 9. Particle Size Distribution of Ground and of Commercial 200-micron AP

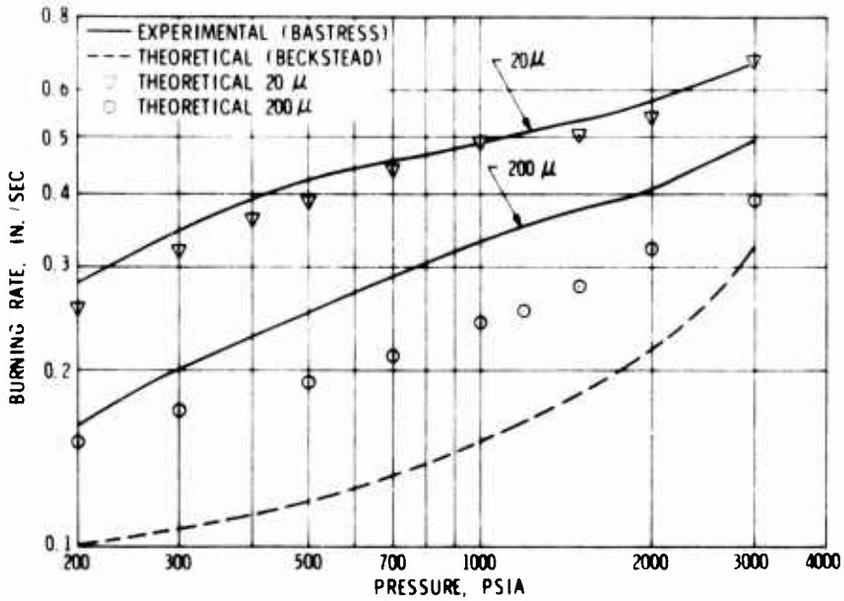

Figure 10. Correlation of Theoretical Burn Rate with Bastress Data for Polysulfide Propellants

CONCLUSIONS

Work completed thus far indicates that a comprehensive and predictive steady-state combustion model of composite solid propellants is possible. These models are complex but modern computing techniques make these models easy to use and study. It is our philosophy in this study to be realistic and include as much known phenomenology of solid propellant combustion as possible but to avoid unnecessary complexity. It is also our purpose to program this model so that it can become a tool for propellant chemists and engineers.

The next step in this program is to add aluminum. The equations have already been written and the treatment will be much the same as is used by Cohen, Derr and Price.[8]

Currently, gas phase conductivities are calculated using Chapman-Enscog theories and then input to the program. Later these calculations will be written into the program.

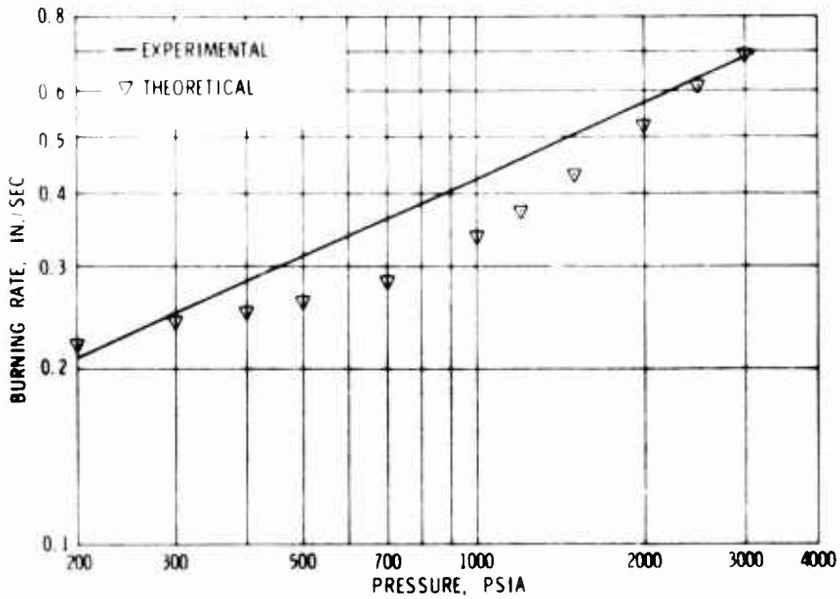

Figure 11. Theoretical Burning Rates for an 84 Percent Oxidizer Loaded Propellant with CTPB Binder

The flame height calculations will be improved by using more terms of the series solution.

Parametric studies run continuously with this program are indicating that the exothermic liquid layer on AP during burning is very important. A treatment should be added based on the surface area of the burning supercritical oxidizer. This surface area is calculated within the program.

The effect of catalyst is to be added by changes in activation energies for the various chemical reactions treated by this model.

REFERENCES

1. Hermance, C. E.: "A Detailed Model of the Combustion of Composite Solid Propellants," proceedings of the ICRPG/AIAA 2nd Sold Propulsion Conference, American Institute of Aeronautics and Astronautics, New York, 1967, pp 89-103.

2. Beckstead, M. W., R. L. Derr and C. F. Price: "A Model of Composite Solid Propellant Combustion based on Multiple Flames," AIAA Journal, Vol 8, No. 9, 2200 (1970).

3. Sammons, G. D.: "Dynamic Calorimetric Solid Propellant Combustion Studies," presented at the AIAA Fifth Propulsion Joint Specialist Conference, Colorado Springs, Colorado, Paper No. 69-504, 9-13 June 1969.

4. Wise, H., S. H. Inami and L. McCulley: "Role of Condensed Phase Reactions in Ignition and Deflagration of Ammonium Perchlorate Propellants," Comb and Flame, Vol 11, 483 (1968).

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6. Schmidt, W. G.: "The Effect of Solid Phase Reactions on the Ballistic Properties of Propellants," NASA contract NAS1-9463, Aerojet Solid Propulsion Company, Report No. NASA CR112083, August 1972.

7. Williams, Foreman: Combustion Theory, Addison-Wesley Publishing Company, Massachusetts, 1965, pp 37-42.

8. Cohen, N. S., R. L. Derr and C. F. Price: "Extended Model of Solid Propellant Combustion Based on Multiple Flames," Postprints from Ninth JANNAF Combustion Meeting.

NOMENCLATURE

T_s	- surface temperature
T_o	- initial propellant temperature
γ	- weight fraction of supercritical AP particles in total propellant
C_p	- specific heat of gas phase
Q_L	- latent heat of vaporization of AP
δ	- weight fraction of binder/critical AP particles consumed in condensed phase reaction
Q_f	- energy of fuel decomposition
Q_s	- energy of condensed phase heat release
β_F	- fraction of reactants reacting in primary flame
ξ_{AP}^*, ξ_{PF}^*, ξ_T	- nondimensional flame standoff distances for monopropellant flame, primary flame and total oxidizer flame

EM 73-05

SOLID PROPELLANT COMBUSTION MODELING

G. D. Sammons

August 1973

Paper presented at 10th JANNAF Combustion Meeting
6--10 August 1973, U.S. Naval War College, Newport,
Rhode Island (presentation made by B. M. Corley).

SOLID PROPELLANT COMBUSTION MODELING

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ABSTRACT

This progress report covers the first 15 months of a continuing study on construction of a comprehensive mathematical model of composite solid propellant combustion, with emphasis on work during the past 12 months since reporting on the early efforts at the meeting last year.

The liquid layer believed to exist on burning ammonium perchlorate has been treated in a manner similar to that described last year. Depth of penetration of a thermal wave is calculated and this value is multiplied by the surface area of oxidizer on the burning propellant surface. The surface is calculated in the computer program for use in other equations. Total volume of the liquid layer derived in this manner is then used to calculate the thermal contribution to surface temperature.

Treatment of aluminum has been added, and the treatment of multimodal oxidizer has been improved. Most internal parameters have been thoroughly checked to verify that they have realistic values. Considerable time was spent on the Burke-Schumann flame height calculations. It has been found that at least seven terms of the series solution must be considered. The single first-term calculations that have been used in the past do not give a good assessment of flame height; the flame height is expressed implicitly in the final equation, and it was necessary to solve it by a Newton-Raphson iteration. Improvement in a number of input parameters is described. Gas phase conductivities were calculated using Chapman-Enskog theories with the Hirschfelder-Eucken corrector. The same theories were used to calculate diffusion coefficients. Stoichiometric ratios were calculated using more realistic pyrolysis species. A thermogravimetric analysis was made of a polybutadiene propellant binder and a statistical method was used to derive kinetic parameters from the thermograms. The method used was the Zsake modification of Doyle's method, which is probably the most sophisticated way of treating TGA data. Some other improvements in programming and correlation with actual propellant motor firings are shown and future plans are given.

INTRODUCTION

Work continued during the past year on the comprehensive modeling of composite solid propellants.* The model being developed is based on the Beckstead, Derr, Price multiflame model (1,2) and utilizes a critical particle size theory (3) to provide a means of calculating condensed phase heat release. A number of improvements have been made to the model and the computer program that was described at the meeting last year (4); one of

*This work is being supported by AFOSR under Contract F44620-72-C-0046.

the major improvements being the addition of a treatment of the liquid layer on burning ammonium perchlorate (AP). These improvements, an example experiment and future plans are described in the following paragraphs.

MATHEMATICAL MODEL AND IMPROVEMENTS

The most recent surface energy balance is shown on Fig. 1. The new terms (not shown last year) are the energy to melt the aluminum and the energy from the liquid layer. In this equation m_{ox} is the mass flux of interstitial propellant; or, more specifically, the binder plus the subcritical AP. The term for condensed phase heat release based on the critical particle size theory is included. The critical particle size theory, stated simply, is that there exists for a given propellant and pressure a particle size where all smaller particles will be consumed in condensed phase reaction. The terms for aluminum fusion and liquid layer on AP are also present. The treatment of aluminum used is somewhat different from that used in the BDP model; with the methodology explained later.

ENERGY TO RAISE PROPELLANT TO T_s	ENERGY TO VAPORIZE OXIDIZER	ENERGY TO VAPORIZE FUEL	ENERGY FROM CONDENSED PHASE	ENERGY TO MELT AL
$m_t c_p (T_s - T_o)$	$= - m_{ox} \frac{S_{ox}}{S_o} Q_L$	$- (1-\delta) m_p \frac{S_p}{S_o} Q_f$	$+ \delta m_p \frac{S_p}{S_o} Q_s$	$- m_{AL} \frac{S_p}{S_o} Q_{AL}$

ENERGY FROM PRIMARY DIFFUSION FLAME	ENERGY FROM AP FLAME	ENERGY FROM FINAL DIFFUSION FLAME	ENERGY FROM AP LIQUID LAYER
$+ \beta_F Q_{PF} m_t \exp\left(-\dot{\xi}_{PF}\right)$	$+ (1-\beta_F) m_{ox} \frac{S_{ox}}{S_o} \left[Q_{AP} \exp\left(\dot{\xi}_{AP}\right) + Q_{FF} \exp\left(\dot{\xi}_T\right) \right]$		$+ \omega m_{ox} \frac{S_{ox}}{S} Q_{LIQ}$

Fig. 1. Critical Particle Size Model Energy Balance

Figure 2 shows first the current equation for surface temperature. This was derived from the energy equation using mass balance equations in the same manner as originally used by Beckstead (2). The following three equations are for the heat release in the primary, final, and AP flames, as denoted by the subscripts (PF, FF, AP).

Flame Heights. The Burke-Schumann equation modified for short flames is shown in Fig. 3. In the past a single term of this expression has been used but we have found that at least seven terms should be used. The equation is really not as complicated as it first appears; it is nothing more than is shown in the second equation. By adding the extra terms the equation has been made implicit in flame height but it is solved easily by a Newton-Raphson iteration. Convergence is obtained rapidly when the initial guess for flame height is taken as one-tenth the value obtained from a single-term calculation. This table is the numerical value of the first five terms; and each term is about half the value of the preceding term. An actual check of flame heights when different numbers of terms are used shows that at least seven terms must be used to get the flame within 1 micron.

SURFACE TEMPERATURE

$$T_s = T_o - \frac{\gamma}{C_p} Q_L - \frac{(1-\delta)(1-\gamma-\epsilon)}{C_p} Q_f + \frac{\delta(1-\gamma-\epsilon)}{C_p} Q_s + \epsilon Q_{AL} + \frac{\beta_F Q_{PF}}{C_p} \exp\left(-\dot{\xi}_{PF}\right) +$$

$$(1-\beta_F)\frac{\gamma}{C_p}\left[Q_{AP} \exp\left(-\dot{\xi}_{AP}\right) + Q_{FF} \exp\left(-\dot{\xi}_T\right)\right] + \frac{\omega\gamma}{C_p} Q_{LIQ}$$

HEAT RELEASE

$$Q_{PF} = C_p (T_f - T_o) + \gamma Q_L + (1-\delta)(1-\gamma-\epsilon) Q_f - \delta(1-\gamma-\epsilon) Q_s + \epsilon Q_{AL} - \omega\gamma Q_{LIQ}$$

$$Q_{FF} = \frac{C_p}{\gamma}\left[(T_f - T_o) - \gamma(T_{AP} - T_o)\right] + \frac{(1-\delta)(1-\gamma-\epsilon)}{\gamma} Q_f - \frac{\delta(1-\gamma-\epsilon)}{\gamma} Q_s + \frac{\epsilon Q_{AL}}{\gamma} - \omega Q_{LIQ}$$

$$Q_{AP} = C_p (T_{AP} - T_o) + Q_L - \omega Q_{LIQ}$$

Fig. 2. Current Equations for Surface Temperature Used in Computer Program

FLAME HEIGHTS

$$\frac{\nu - (1+\nu) C^2}{2(1+\ ) C} = \sum_{n=1}^{\infty} \frac{1}{\phi n} \frac{J_1 (C\phi n)}{\left[J_o (\phi n)\right]^2} \exp\left[-\frac{\left(\left[1 + (2\psi\phi_n)^2\right]^{\frac{1}{2}} - 1\right)}{2\psi^2} \eta\right]$$

$$A = B_1 \exp(-C_1\eta) + B_2 \exp(-C_2\eta) + \ldots B_n \exp(-C_n\eta)$$

SIZE OF TERMS

1 - 0.072
2 - 0.046
3 - 0.024
4 - 0.011
5 - 0.005

SOLVED BY NEWTON-RAPHSON ITERATION

$$\eta_{n+1} = \eta_n - \frac{f(x)}{f'(x)}$$

Fig. 3. Burke-Schumann Equation Modified for Short Flames

A number of other improvements have been made to the computer program for this model. During the past year all parameters have been thoroughly checked, particularly those used internally and normally not listed. We found that some of the volume and weight fractions would become unrealistic; e.g., greater than one. When this occurred it caused discontinuities in the burn rate curve. This was remedied by setting boundaries on these parameters.

Treatment of the oxidizer particle size has been improved. The spline fit of the particle size distribution curve is still used. A normal bi- or tri-modal oxidizer blend will usually be split into 10 modes by this technique. Calculation of the h/D ratios is handled in a different manner than that described by Cohen, Derr, and Price (5) last year (Fig. 4). Each mode of supercritical oxidizer is split into 50 parts; the ignition delay term in the equation for h/D is calculated for each part, summed and averaged. Each ignition term is then multiplied by the weight fraction of the mode and summed with similar terms produced from each mode. Then h/D and S_{ox} are calculated.

SURFACE DIMENSIONALITY

$$\frac{h}{D} = \frac{1}{2}\left(1 \pm \sqrt{\frac{1}{3}}\right)\left(1 - \frac{r_{ox}}{r_f}\right) + r_{ox}\frac{K_o D^n}{P^m}$$

DIFFUSION COEFFICIENT

$$D_{AB} = \frac{C\sqrt{T^3\left(\frac{1}{M_A} + \frac{1}{M_B}\right)}}{P\,\sigma_{AB}^2\,\Omega_{AB}}$$

LIQUID LAYER TREATMENT

$$\omega = \frac{S_{ox}}{S}\frac{D_c}{\gamma}\frac{\rho_{ox}}{\rho_p}$$

Fig. 4. Calculations for h/D Ratios

Oxidizer/fuel stoichiometric ratios are different in the primary flame and the final flame. At temperatures such as are found at the binder surface it is known that polybutadiene depolymerizes (6) with the major specie produced being butadiene. This is considered the major diffusing specie in the primary flame, giving a stoichiometric ratio of 3.7. The Chapman-Enskog equation in the center of Fig. 4 was then used to calculate the diffusion coefficient for the primary flame. In the final flame it was assumed that hydrocarbon fragments were the major diffusing species; a stoichiometric ratio of 8.0 was used, along with a larger diffusion coefficient.

Liquid Layer. The AP liquid layer was not treated as a melt but as an exothermic layer. We have always assumed this layer to be a solution of

AP and perchloric acid. A thermal wave penetration is calculated in the same manner as for the critical particle size. This volume is converted to weight fraction of AP in the propellant that is available for exothermic surface reaction (Ref equation at bottom of Fig. 4).

EXPERIMENTAL RESULTS

The combustion model with the improvements noted above was applied to several smokeless propellants for which experimental data were available. Theoretical calculations for three of the propellants (based on carboxy-terminated polybutadiene binders) were made at two initial propellant temperatures and temperature sensitivities of burning rates were calculated. As shown in Table I, agreement of 77 F burn rates is good. Slopes of the burn rate curves are identical. The σ_k values were calculated using the one over one minus "n" relationship. The theoretical σ_k values are all low and should be two to three times higher; and we will look into this further.

Table I. Temperature Sensitivity

EXPERIMENTAL				THEORETICAL			
r at 1000 psi, in./sec	Slope	σ_p, %/deg F	σ_k, %/deg F	r at 1000 psi in./sec	Slope	σ_p, %/deg F	σ_k, %/deg F
0.43	0.38	0.10	0.16	0.38	0.36	0.04	0.06
0.29	0.50	0.07	0.13	0.27	0.50	0.02	0.05
0.45	0.50	0.10	0.21	0.40	0.50	0.03	0.07

Figure 5 shows a burning rate vs pressure plot; the upper line represents a least squares fit to rocket motor firings; the lower line, the theoretical. This is a two cycle-by-two cycle log-log plot. The scales are the same as those widely used in industry to plot rocket motor rate; therefore, the data are presented in a realistic, practical manner. As noted last year we did not use strand data for correlative purposes since strand rates are not necessarily predictive of motor rates. Propellant used in the motor from which the plotted data were taken has a Butarez CTL-type binder and an 86% solids loading. The trimodal oxidizer is comprised of commercial 200- and 80-micron fractions and Majac-ground

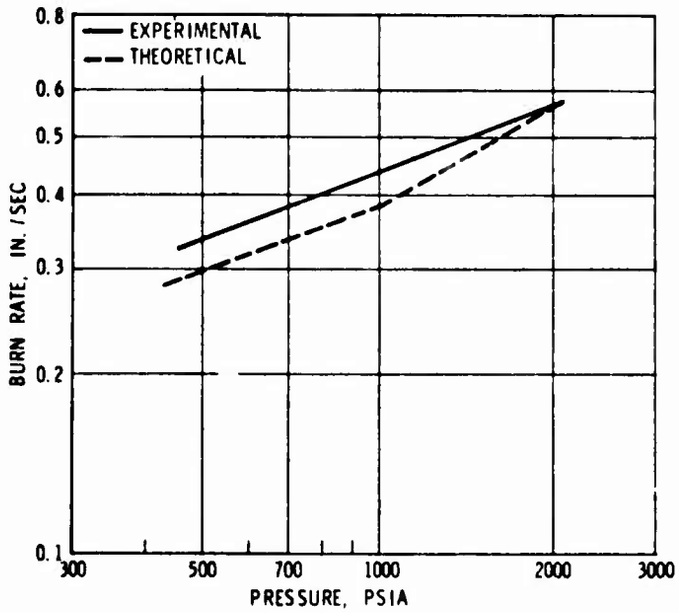

Fig. 5. Propellant with Butarez CTL Type with 86% Solids and Trimodal Oxidizer

10-micron AP at weight percent levels 35/26/25. The theoretical curve is identical in slope up to 1000 psi.

Comparable data with a propellant containing a trimodal mixture of 400-, 200-, and 80-micron AP at weight percent levels 51/20/15, respectively, are shown in Fig. 6. The break at 1000 psi is well verified by motor firings. No curve fitting was used to obtain these results; i.e., they were obtained on the first computer run. Fig. 7 shows data from a hydroxy-terminated polybutadiene (HTPB)-based propellant with a large amount of fine oxidizer; i.e., a trimodal blend of 200-, 80-, and 10-micron at weight percent levels of 31/15/40, respectively. Again, we are comparing motor data; and, although the burn rate is somewhat lower, the two lines have identical slopes. Data from a propellant that has a tetramodal oxidizer, i.e., 400-, 200-, 80-, and 10-micron at weight percent levels of 56/13/12/5, respectively, are shown in Fig. 8. We would like to emphasize again that no manipulation of parameters was required; the curve represents the first run made for the oxidizer blend with the current computer program.

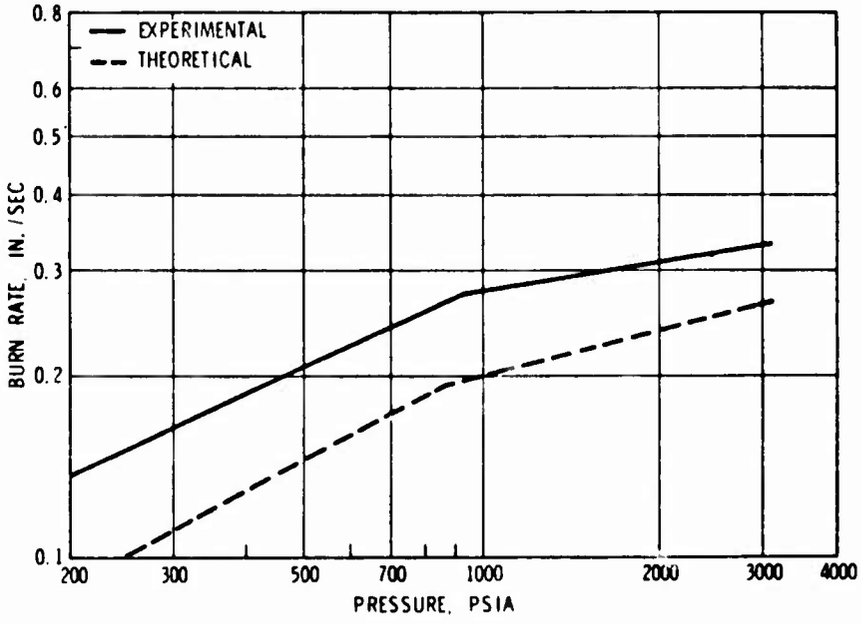

Fig. 6. Propellant with Butarez CTL Type Binder with 86% Solids and Trimodal Oxidizer

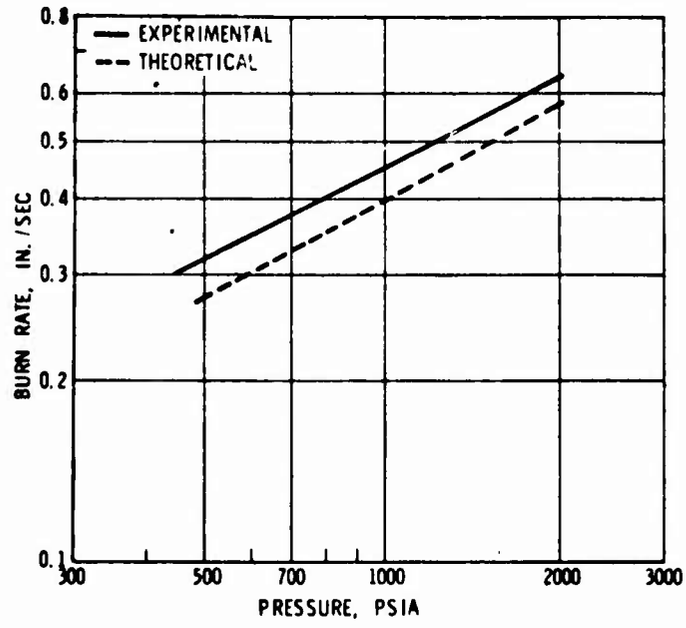

Fig. 7. Propellant with HTPB-Type Binder with 86% Solids and Trimodal Oxidizer

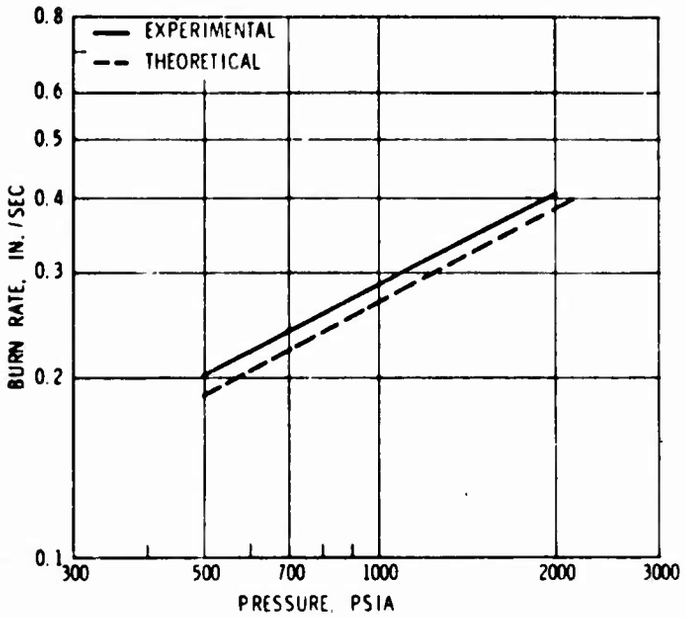

Fig. 8. Propellant with HTPB-Type Binder with 86% Solids and Trimodal Oxidizer

FUTURE PLANS

In the ensuing months, we plan to further study the possibilities of a two surface temperature model, add a treatment for the catalyst, and continue studying the effects of particle size. We will also establish possible maximum and minimum burn rates and continue to make improvements in the computer program.

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1. Hermance, C. E.: "A Detailed Model of the Combustion of Composite Solid Propellants," proceedings of the ICRPG/AIAA 2nd Solid Propulsion Conference, American Institute of Aeronautics and Astronautics, New York, 1967, pp 89-103.

2. Beckstead, M. W., R. L. Derr and C. F. Price: "A Model of Composite Solid Propellant Combustion based on Multiple Flames," AIAA Journal, Vol 8 No. 9, 2200 (1970).

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4. Sammons, G. D.: "Advancement of Comprehensive Combustion Modeling," 9th JANNAF Combustion Meeting, CPIA Pub. 231, December 1972, 43.

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APPENDIX II

COMPUTER PRINTOUT OF THE PROGRAM NRCOMB

FORTRAN MODULE (LIST)

CARD NO **** CONTENTS ****

```
      C     MAIN NRCOMB 10-11-72 VERSION                                    00100010
      C                                                                     00100020
            COMMON  A1,     A2,     AF,     AFH,    ALFA,   RHAL          00100030
            COMMON  AOX,    BESS,   BETAF,  BSQR,   C3P                   00100040
            COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO         00100050
            COMMON  EF,     FOX,    ETA,    GAMMA,  GMW,    HON           00100060
            COMMON  HOP,    IJIM,   IPLOT,  K,      KAP1,   KAP2          00100070
            COMMON  KPF,    EPS,    MOX,    MT,     NP1,    P             00100080
            COMMON  POWD,   POWIGN, PSTART, PSTOP,  QAP,    QFF           00100090
            COMMON  QFUEL,  QL,     QPF,    R,      RAP,    RF            00100100
            COMMON  RHOF,   RHOP,   RHOX,   RON,    SOX,    TAP           00100110
            COMMON  TAV,    TF,     TIT1(20),TZERO, TS                    00100120
            COMMON  XLAMB,  XN1,    XN2,    XN3,    XNU,    XNU1          00100130
            COMMON  XSTAP,  XSTARD, XSTPD,  XSTPF,  XNUP,   ETAP          00100140
            COMMON  PMW,    IPLT,   GAM,    DEL,    XNUU,   WAP           00100150
            COMMON  PR1,    PR2,    PR3,    PR4,    PR6,    PR7           00100160
            COMMON PR8                                                    00100170
            COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)           00100180
            COMMON NN,RHOPI,XNUSC,RON1,RONN                               00100190
            COMMON CZERO,SIGC,CPIT,QSOLID                                 00100200
            COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                         00100210
            COMMON AFH1,ME,XSPD,XSAP,ISI                                  00100220
            COMMON C25(20),NJOB,IJX                                       00100230
            COMMON SII(20),QLIQ                                           00100240
            COMMON INI,M1                                                 00100250
            COMMON QAL                                                    00100260
      C                                                                   00100270
            REAL KAP1,KAP2,KPF,MOX,MT                                     00100280
            INTEGER AH                                                    00100290
            A1=0.5*(1.+1./SQRT(3.))                                       00100300
            A2=0.5*(1.-1./SQRT(3.))                                       00100310
            RN=.001                                                       00100320
      2     AH=0                                                          00100330
            IJX=1                                                         00100340
            IX=1                                                          00100350
            CRIT=10.                                                      00100360
            ISI=0.0                                                       00100370
            IJIM=0                                                        00100380
            CALL INPUT1                                                   00100390
            AFH1=AFH                                                      00100400
            INI=0                                                         00100410
            CALL CONCAL                                                   00100420
            K=1                                                           00100430
            R=.06*SQRT(P)                                                 00100440
            SOX=XNU                                                       00100450
      9     CALL CONVR                                                    00100460
      33    M1=1                                                          00100470
```

```
      CALL OUTPUT                                                       00100480
      IF(P-PSTOP)31,32,32                                               00100490
31    INI=1                                                             00100500
      CALL CONCAL                                                       00100510
8     CONTINUE                                                          00100520
      GO TO 9                                                           00100530
32    M1=2                                                              00100540
      CALL OUTPUT                                                       00100550
      GO TO 2                                                           00100560
      END                                                               00100570
      SUBROUTINE INPUT1                                                 00200010
C                                                                       00200020
      COMMON  A1,     A2,     AF,     AFH,    ALFA,   BHAL            00200030
      COMMON  AOX,    BESS,   BETAF,  BSQR,   C3P                     00200040
      COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO           00200050
      COMMON  EE,     EOX,    ETA,    GAMMA,  GMW,    HON             00200060
      COMMON  HOP,    IJIM,   IPLOT,  K,      KAP1,   KAP2            00200070
      COMMON  KPF,    FPS,    MOX,    MT,     NP1,    P               00200080
      COMMON  POWD,   POWIGN, PSTART, PSTOP,  QAP,    QEF             00200090
      COMMON  QFUEL,  QL,     QPF,    R,      RAP,    PF              00200100
      COMMON  RHOF,   RHOP,   RHOX,   RON,    SOX,    TAP             00200110
      COMMON  TAV,    TF,     TIT1(20), TZERO, TS                     00200120
      COMMON  XLAMB,  XN1,    XN2,    XN3,    XNU,    XNU1            00200130
      COMMON  XSTAP,  XSTARD, XSTPD,  XSTPF,  XNUP,   ETAP            00200140
      COMMON  PMW,    IPLT,   GAM,    DEL,    XNUU,   WAP             00200150
      COMMON  PR1,    PR2,    PR3,    PR4,    PR6,    PR7             00200160
      COMMON PRR                                                        00200170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)               00200180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                   00200190
      COMMON CZERO,SIGC,CRIT,QSOLID                                     00200200
      COMMON SIGSC,IX,LLL,PN,AH,C10,C15,C20                             00200210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                      00200220
      COMMON C25(20),NJOB,IJX                                           00200230
      COMMON SII(20),QLIQ                                               00200240
      COMMON INI,M1                                                     00200250
      COMMON OAI                                                        00200260
C                                                                       00200270
      REAL KAP1,KAP2,KPF,MOX,MT                                         00200280
      INTEGER AH                                                        00200290
C                                                                       00200300
      DATA XEND/'END '/                                                 00200310
C                                                                       00200320
      ISI=1                                                             00200330
    1 READ (5,800) TIT1                                                 00200340
  800 FORMAT(20A4)                                                      00200350
      IF(TIT1(1).NE.XEND) GO TO 16                                      00200360
      CALL EXIT                                                         00200370
      STOP                                                              00200380
   16 READ (5,100) NJOB , IPLOT , IPLT                                  00200390
  100 FORMAT(12I6)                                                      00200400
      IF(NJOB.EQ.100)GO TO 13                                           00200410
      IF(NJOB.EQ.105)GO TO 11                                           00200420
      GO TO 12                                                          00200430
   13 M1 = 2                                                            00200440
      CALL OUTPUT                                                       00200450
      GO TO 1                                                           002  460
```

```
104             12    GO TO (2,3,4,5,6,7,8,9,10,11,20),NJOB                                    00200470
105                2 READ (5,810) TZERO , ALFA  , TF    , GMW   , XNU1  , DZERO                00200480
106                  READ (5,810) QFUEL , RHOF  , AF    , EF    , XNUP  , PMW                  00200490
107                  READ (5,810) QL    , RHOX  , AOX   , EOX   , TAP                          00200500
108                  READ (5,810) CIGN  , POWIGN, POWD  , PSTART, PSTOP                        00200510
109                  READ (5,810) KPF   , KAP1  , KAP2  , XN1   , XN2   , XN3                  00200520
110                  READ (5,810) CSUBP , XLAMB , GAMMA , AFH                                  00200530
111                  READ(5,810) TS , QSOLID , QLIQ , QAL , RHAL                               00200540
112               810 FORMAT(6E12.5)                                                           00200550
113                   GO TO (10,30),ISI                                                       00200560
114             30    CALL OXID1(1)                                                           00200570
115                   GO TO 11                                                                00200580
116                3 READ (5,810) AF    , AOX                                                 00200590
117                  GO TO 11                                                                00200600
118                4 READ (5,810) QL                                                         00200610
119                  GO TO 11                                                                00200620
120                5 READ (5,810) XNU1                                                       00200630
121                  GO TO 11                                                                00200640
122                6 READ (5,810) AFH                                                        00200650
123                  GO TO 11                                                                00200660
124                7 READ (5,810) PSTART,PSTOP                                             00200670
125                  GO TO 11                                                                00200680
126                8 READ (5,820) IX    ,TZERO                                               00200690
127               820 FORMAT(I6,6X,E12.5)                                                    00200700
128                   GO TO 11                                                                00200710
129                9 READ (5,810) QFUEL                                                      00200720
130                  GO TO 11                                                                00200730
131             10    CONTINUE                                                                00200740
132                   READ (5,100) NN                                                         00200750
133                   READ (5,810) (SIG(J),DMIN(J),DMAX(J),J=1,NN)                            00200760
134                   CALL OXID1(1)                                                           00200770
135                   READ (5,810) EPS                                                        00200780
136                   GO TO 11                                                                00200790
137             20    EPS=0.0                                                                 00200800
138                   SIG(1)=.09394                                                           00200810
139                   SIG(2)=.24096                                                           00200820
140                   SIG(3)=.233                                                             00200830
141                   SIG(4)=.11038                                                           00200840
142                   SIG(5)=.09692                                                           00200850
143                   SIG(6)=.12269                                                           00200860
144                   SIG(7)=.05543                                                           00200870
145                   SIG(8)=.02918                                                           00200880
146                   SIG(9)=.0175                                                            00200890
147                   DMIN(1)=230.                                                            00200900
148                   DMIN(2)=140.                                                            00200910
149                   DMIN(3)=78.                                                             00200920
150                   DMIN(4)=35.                                                             00200930
151                   DMIN(5)=12.                                                             00200940
152                   DMIN(6)=4.8                                                             00200950
153                   DMIN(7)=2.5                                                             00200960
```

CARD NO **** CONTENTS ****

```
      DMIN(8)=1.2                                                                00200970
      DMIN(9)=.3                                                                 00200980
      DMAX(1)=500.                                                               00200990
      DMAX(2)=230.                                                               00201000
      DMAX(3)=140.                                                               00201010
      DMAX(4)=78.                                                                00201020
      DMAX(5)=35.                                                                00201030
      DMAX(6)=12.                                                                00201040
      DMAX(7)=4.8                                                                00201050
      DMAX(8)=2.5                                                                00201060
      DMAX(9)=1.2                                                                00201070
      ALFA=86.                                                                   00201080
      ME=0                                                                       00201090
      QSOLID=1085                                                                00201100
      ISI=2                                                                      00201110
      NN=9                                                                       00201120
11    CONTINUE                                                                   00201130
      XNU=1./(1.+EPS*RHOX/(ALFA*RHAL)+RHOX*(1.-ALFA-EPS)/(RHOF*                  00201140
     &ALFA))                                                                     00201150
      IF(XNU.GT.1.)XNU=1.0                                                       00201160
      TAV=(TAP+TF)/2.                                                            00201170
      RETURN                                                                     00201180
      END                                                                        00201190
      SUBROUTINE OUTPUT                                                          00300010
C                                                                                00300020
      COMMON   A1,     A2,       AF,       AFH,    ALFA,    RHAL                00300030
      COMMON   AOX,    BESS,     BETAF,  BSQR,     C3P                         00300040
      COMMON   C4P,    CIGN,     CON1,     CSUBP,  DELDI,   DZERO               00300050
      COMMON   EF,     EOX,      ETA,      GAMMA,  GMW,     HON                 00300060
      COMMON   HOP,    IJIM,     IPLOT,    K,      KAP1,    KAP2                00300070
      COMMON   KPF,    EPS,    MOX,      MT,     NP1,     P                   00300080
      COMMON   POWD,   POWIGN,   PSTART,   PSTOP,  QAP,     QFF                 00300090
      COMMON   QFUEL,  QL,       QPF,      R,      RAP,     RF                  00300100
      COMMON   RHOF,   RHOP,     RHOX,     RON,    SOX,     TAP                 00300110
      COMMON   TAV,    TF,       TIT1(20), TZERO,  TS                          00300120
      COMMON   XLAMB,  XN1,      XN2,      XN3,    XNU,     XNU1                00300130
      COMMON   XSTAP,  XSTARD,   XSTPD,    XSTPF,  XNUP,    ETAP                00300140
      COMMON   PMW,    IPLT,     GAM,      DEL,    XNUU,    WAP                 00300150
      COMMON   PR1,    PR2,      PR3,      PR4,    PR6,     PR7                 00300160
      COMMON PR8                                                                 00300170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)                        00300180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                            00300190
      COMMON CZERO,SIGC,CRIT,QSOLID                                              00300200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                                      00300210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                               00300220
      COMMON C25(20),NJOB,IJX                                                    00300230
      COMMON SII(20),QLIQ                                                        00300240
      COMMON IN1,M1                                                              00300250
      COMMON QAL                                                                 00300260
C                                                                                00300270
```

```
204                 REAL KAP1,KAP2,KPF,MOX,MT                                   00300280
205                 DIMENSION BR(30),PT(30),ST(30),HDP1(30),HDN1(30),BRA(30)    00300290
206                 DIMENSION PTA(30),MOX1(30),SOX1(30),XST1(30),XST2(30)       00300300
207                 DIMENSION CTL(30)                                           00300310
208                 DIMENSION XST3(30),XST4(30),BET1(30)                        00300320
209                 DIMENSION PTAL(30),BRAL(30)                                 00300330
210                 REAL MOX1                                                   00300340
211                 INTEGER AH                                                  00300350
212                 DATA IYES/'YES '/                                           00300360
213                 GO TO (10,20),M1                                            00300370
214           10    BR(K)=R                                                     00300380
215           C     WRITE(6,204) K,RONN                                         00300390
216           C     WRITE(6,205) PAP                                            00300400
217           C     WRITE(6,205) RF                                             00300410
218           C 204 FORMAT(5X,I3,5X,F12.5)                                      00300420
219           C 205 FORMAT(10X,F7.3)                                            00300430
220                 PT(K)=P                                                     00300440
221                 ST(K)=TS-273.2                                              00300450
222                 HDP1(K)=HDP                                                 00300460
223                 HDN1(K)=HDN                                                 00300470
224                 BRA(K)=BR(K)/2.54                                           00300480
225                 PTA(K)=PT(K)*14.7                                           00300490
226                 MOX1(K)=MOX                                                 00300500
227                 SOX1(K)=SOX                                                 00300510
228                 XST1(K)=XSTPD*10000.                                        00300520
229                 XST2(K)=XSTPF*10000.                                        00300530
230                 XST3(K)=XSTAP*10000.                                        00300540
231                 XST4(K)=XSTARD*10000.                                       00300550
232                 CTL(K)=CRIT                                                 00300560
233                 BET1(K)=BETAF                                               00300570
234           1     CALL ENERGY(1,0,0,0,0)                                      00300580
235           7     CALL FACTOR(1,0,0,0,0,0)                                    00300590
236                 SQPSI=C20                                                   00300600
237           C     CALL FLAHT(1,0,0,SQPSI,0)                                   00300610
238           8     CONTINUE                                                    00300620
239           9     CONTINUE                                                    00300630
240                 IF(SIGC.GT.0.0)ISI=1                                        00300640
241           C     WRITE(6,210) AFH,AFH1                                       00300650
242           C 210 FORMAT(10X,'AFH= ',E15.8,5X,'AFH1= ' E15.8)                 00300660
243                 KMAX=K                                                      00300670
244                 K=K+1                                                       00300680
245                 RETURN                                                      00300690
246              20 IF(NJOB.EQ.105)GO TO 150                                    00300700
247                 GO TO (13,3,16,17,18,19), IX                                00300710
248           13    IF(PSTART.EQ.PSTOP)GO TO 70                                 00300720
249                 WRITE(6,101) TIT1                                           00300730
250                 GO TO 19                                                    00300740
251           17    CONTINUE                                                    00300750
252                 GO TO 50                                                    00300760
253           18    CONTINUE                                                    00300770
254           C     18 CALL FLAHT(2,PTA,BRA,0,KMAX)                             00300780
255                 RETURN                                                      00300790
256           19    CONTINUE                                                    00300800
257                 XNUT=ALFA*100.                                              00300810
258                 TZIP=TZERO-273.                                             00300820
259                 IF(IPLT)6,11,6                                              00300830
```

```
      3     CALL ENERGY(2,PTA,BRA,CTL,KMAX)                                   00300840
            RETURN                                                            00300850
     16     CALL FACTOR(2,PTA,BRA,BET1,CTL,KMAX)                              00300860
            RETURN                                                            00300870
      6     CONTINUE                                                          00300880
            WRITE(10)KMAX                                                     00300890
            DO 4 K=1,KMAX                                                     00300900
            PTAL(K)=ALOG10(PTA(K))                                            00300910
            BRAL(K)=ALOG10(BRA(K))                                            00300920
      4     WRITE(10)PTAL(K),BRAL(K)                                          00300930
            IF(IPLT.EQ.2) RETURN                                              00300940
     11     CONTINUE                                                          00300950
            IF (IPLOT)15,15,40                                                00300960
     15     CONTINUE                                                          00300970
            WRITE(6,140)                                                      00300980
            WRITE(6,107) XNUT , DZERO                                         00300990
            WRITE(6,106) DELDI, RHOP                                          00301000
            WRITE(6,108) RHOF , RHOX                                          00301010
            WRITE(6,109) QFUEL, TF                                            00301020
            WRITE(6,110) GMW  , PMW                                           00301030
            WRITE(6,111) GAMMA, BESS                                          00301040
            WRITE(6,112) XNU1 , XNUP                                          00301050
            WRITE(6,145)                                                      00301060
            WRITE(6,113) CIGN , POWIGN                                        00301070
            WRITE(6,114) POWD , QL                                            00301080
            WRITE(6,154)                                                      00301090
            WRITE(6,115) EF   , EOX                                           00301100
            WRITE(6,116) AF   , AOX                                           00301110
            WRITE(6,117) XN1  , KPF                                           00301120
            WRITE(6,118) XN2  , KAP1                                          00301130
            WRITE(6,119) XN3  , KAP2                                          00301140
            WRITE(6,155)                                                      00301150
            WRITE(6,120) TAP  , XLAMB                                         00301160
            WRITE(6,121) CSUBP, QFF                                           00301170
            WRITE(6,122) QPF  , AFH                                           00301180
            WRITE(6,123) TZIP                                                 00301190
     40     CONTINUE                                                          00301200
            READ (5,134) IAN                                                  00301210
            IF(IAN.EQ.IYES) GO TO 70                                          00301220
            WRITE(6,124)                                                      00301230
            DO 69 K=1,KMAX                                                    00301240
            WRITE(6,125) PT(K), PTA(K), BR(K), BRA(K), ST(K), CTL(K)          00301250
     69     CONTINUE                                                          00301260
            WRITE(6,160)                                                      00301270
            WRITE(6,129)                                                      00301280
            DO 50 K=1,KMAX                                                    00301290
            WRITE(6,126) PT(K),HDP1(K),HDN1(K),MOX1(K),SOX1(K)                00301300
     50     CONTINUE                                                          00301310
            WRITE(6,160)                                                      00301320
            WRITE(6,127)                                                      00301330
```

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CARD NO    ****                       CONTENTS                                   ****

           DO 68 K=1,KMAX                                                   00301340
     68    WRITE(6,128)PTA(K), BRA(K),XST1(K),XST2(K),XST3(K),XST4(K)       00301350
           GO TO 30                                                         00301360
     70    IF(ISI.EQ.0)  GO TO 72                                           00301370
           WRITE(6,130)                                                     00301380
           DO 71 K=1,KMAX                                                   00301390
           WRITE(6,131)PTA(K), BRA(K), CTL(K)                               00301400
     71    CONTINUE                                                         00301410
           GO TO 30                                                         00301420
     72    WRITE(6,132)                                                     00301430
           DO 73 K=1,KMAX                                                   00301440
           WRITE(6,133)PTA(K), BRA(K)                                       00301450
     73    CONTINUE                                                         00301460
           GO TO 30                                                         00301470
    150    WRITE(6,151)                                                     00301480
           DO 152 K=1,KMAX                                                  00301490
           WRITE(6,153)HDN1(K),HDP1(K),SOX1(K)                              00301500
    152    CONTINUE                                                         00301510
    30     CONTINUE                                                         00301520
    C                                                                       00301530
      151 FORMAT(8X'HDN'8X'HDP'8X'SOX'/)                                    00301540
      153 FORMAT(1X,2F11.4,2X,F7.4)                                         00301550
      101 FORMAT(1H1//20A4//)                                               00301560
      107 FORMAT(6X'WT PERCENT OXID =',F6.1,6X'MEAN DIAM OF',F6.1,' MICRON')00301570
      106 FORMAT(6X'DELDI =',F7.4,15X,'PROP DENSITY =',F5.2)                00301580
      108 FORMAT(6X'BINDER DENSITY =',F5.2,8X'OXID DENSITY=',F5.2)          00301590
      109 FORMAT(5X'QFUEL =',F6.1,16X'TF(DEG K) =',F6.0)                    00301600
      110 FORMAT(6X'MOL WT =',F6.2,15X'PRI MOL WT =',F6.2)                  00301610
      111 FORMAT(6X'DIFF PARAM =',E11.4,6X'BESS FUNCT =',F7.4)              00301620
      112 FORMAT(6X'ST RAT =',F6.2,15X'PRI ST RAT =',F6.2//)                00301630
      113 FORMAT(6X'CIGN =',F6.1,17X'POWIGN =',F6.3)                        00301640
      114 FORMAT(5X'POWD =',F6.1,17X'LATENT HEAT =',F7.1//)                 00301650
      115 FORMAT(6X'EF =',F8.0,17X'E OX =',F8.0)                            00301660
      116 FORMAT(5X'AF =',E10.3,15X'A OX =',E10.3)                          00301670
      117 FORMAT(6X'ORDER,PF =',F6.3,13X'RT CON, PF =',E10.3)               00301680
      118 FORMAT(6X'ORDER,LP =',F6.3,13X'RT CON, LP =',E10.3)               00301690
      119 FORMAT(6X'ORDER,HP =',F6.3,13X'RT CON, HP =',E10.3//)             00301700
      120 FORMAT(6X'OXID FLM TEMP =',F7.1,7X'GAS CONDUCT =',F8.5)           00301710
      121 FORMAT(6X'CP(AVE) =',F7.4,13X'QFF =',F7.1)                        00301720
      122 FORMAT(6X'QPF =',F7.1,17X'AV FLM HT FACT =',F7.4//)               00301730
      123 FORMAT(1X'PROPELLANT INITIAL TEMP IS',F6.1,' DEG CENTIGRADE'//)   00301740
      124 FORMAT(1H1/2X'PT ATMS'5X'PT, PSIA'5X'BR, CM/SEC'4X'BR, IN/SEC'    00301750
         *         3X'SURF T'7X'CRIT'//)                                    00301760
      125 FORMAT(F9.2,F12.1,F15.4,F13.4,F12.2,F9.3)                         00301770
      126 FORMAT(F9.2,4F13.4)                                               00301780
      127 FORMAT(1H1/1X'PT, PSIA'3X'BR, IN/SEC   XTAR PD    XTAR PF'        00301790
         *         4X'XTAR AP    XTAR D'//)                                 00301800
      128 FORMAT(F9.1,F10.4,1X,4F11.2)                                      00301810
      129 FORMAT(2X'  PT ATM           HDP'10X'HDN'10X'MOX'10X'SOX'//)      00301820
      130 FORMAT(1H1/2X'PT, PSIA'4X'BR IN/SEC'4X'CRIT'//)                   00301830
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  131 FORMAT(F9.1,F14.4,F12.3)                                         00301840
  132 FORMAT(1H1/2X'PT, PSIA'4X'BR IN/SEC'//)                          00301850
  133 FORMAT(F9.1,F14.4)                                               00301860
  134 FORMAT(A4)                                                       00301870
  140 FORMAT(1H0/ 20X'PROPELLANT DATA IS'//)                           00301880
  145 FORMAT(1H0//13X'OXIDIZER IGNITION AND BURNING DATA IS'//)        00301890
  154 FORMAT(1H0//12X'ACTIVATION ENERGIES AND RATE FACTORS ARE'//)     00301900
  155 FORMAT(1H0//20X'FLAME PROPERTIES ARE'//)                         00301910
  160 FORMAT(1H0////)                                                  00301920
C                                                                      00301930
      RETURN                                                           00301940
      END                                                              00301950
      SUBROUTINE ENERGY(I,PTA,BRA,CTL,KMAX)                            00400010
C                                                                      00400020
      COMMON  A1,     A2,      AF,       AFH,     ALFA,    RHAL        00400030
      COMMON  AOX,    BESS,    BETAF, BSQR,   C3P                      00400040
      COMMON  C4P,    CIGN,    CON1,     CSUBP,   DELDI,   DZERO       00400050
      COMMON  EF,     EOX,     ETA,      GAMMA,   GMW,     HDN         00400060
      COMMON  HDP,    IJIM,    IPLOT,    K,       KAP1,    KAP2        00400070
      COMMON  KPF,    EPS,    MOX,      MT,      NP1,     P            00400080
      COMMON  POWD,   POWIGN,  PSTART,   PSTOP,   QAP,     QFF         00400090
      COMMON  QFUEL,  QL,      QPF,      R,       RAP,     RF          00400100
      COMMON  RHOF,   RHOP,    FHOX,     RON,     SOX,     TAP         00400110
      COMMON  TAV,    TF,      TIT1(20), TZERO,   TS                   00400120
      COMMON  XLAMB,  XN1,     XN2,      XN3,     XNU,     XNU1        00400130
      COMMON  XSTAP,  XSTARD,  XSTPD,    XSTPF,   XNUP,    ETAP        00400140
      COMMON  PMW,    IPLT,    GAM,      DFL,     XNUU,    WAP         00400150
      COMMON  PR1,    PR2,     PR3,      PR4,     PR6,     PR7         00400160
      COMMON  PR8                                                      00400170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)              00400180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                  00400190
      COMMON CZERO,SIGC,CRIT,QSOLID                                    00400200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                            00400210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                     00400220
      COMMON C25(20),NJOB,IJX                                          00400230
      COMMON SII(20),QLIQ                                              00400240
      COMMON INI,M1                                                    00400250
      COMMON QAL                                                       00400260
C                                                                      00400270
      DIMENSION PA(30),PB(30),PC(30),PD(30),PE(30),PF(30)              00400280
      DIMENSION PTA(30),BRA(30)                                        00400290
      DIMENSION CTL(30),PG(30)                                         00400300
      GO TO (1,2),I                                                    00400310
    1 PA(K)=PR1                                                        00400320
      PB(K)=PR2                                                        00400330
      PC(K)=PR3                                                        00400340
      PD(K)=PR4                                                        00400350
      PE(K)=PR6                                                        00400360
      PF(K)=PR7                                                        00400370
      PG(K)=PR8                                                        00400380
      RETURN                                                           00400390
    2 CONTINUE                                                         00400400
      WRITE(6,3)                                                       00400410
      DO 4 J=1,KMAX                                                    00400420
      WRITE(6,8) PTA(J), BRA(J), PA(J) , PB(J) , PC(J) , CTL(J)        00400430
    4 CONTINUE                                                         00400440
```

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      WRITE(6,160)                                                          00400450
      WRITE(6,5)                                                            00400460
      DO 7 J=1,KMAX                                                         00400470
      WRITE(6,6) PTA(J), PG(J) , PD(J) , PE(J) , PF(J) , CTL(J)             00400480
7     CONTINUE                                                              00400490
      RETURN                                                                00400500
    3 FORMAT(2X'PT, PSIA'4X'BR, IN/SEC'3X'OXID VAP'5X'FUEL VAP'             00400510
     *       5X'CP HEAT'6X'CRIT'//)                                         00400520
    8 FORMAT(F9.1,F14.4,F12.1,2F13.1,F13.2)                                 00400530
    5 FORMAT(2X'PT, PSIA'4X'QLIQ'9X'OFHEAT'6X'APFHEAT'5X'FFHEAT'            00400540
     *       6X'CRIT'//)                                                    00400550
    6 FORMAT(F9.1,4F11.1,F11.3)                                             00400560
  160 FORMAT(1H0////)                                                       00400570
      END                                                                   00400580
      SUBROUTINE FACTOR(I,PTA,BRA,BETI,CTL,KMAX)                            00500010
C                                                                           00500020
      COMMON  A1,     A2,     AF,     AFH,    ALFA,   RHAL                  00500030
      COMMON  AOX,    BESS,   BETAF, BSOR,    C3P                           00500040
      COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO                 00500050
      COMMON  FF,     FOX,    ETA,    GAMMA,  GMW,    HDN                   00500060
      COMMON  HDP,    IJIM,   IPLOT,  K,      KAP1,   KAP2                  00500070
      COMMON  KPF,    EPS,    MOX,    MT,     NP1,    P                     00500080
      COMMON  POWD,   POWIGN, PSTART, PSTOP,  QAP,    QFF                   00500090
      COMMON  QFUEL,  QL,     QPF,    R,      RAP,    RF                    00500100
      COMMON  RHOF,   RHOP,   RHOX,   RON,    SOX,    TAP                   00500110
      COMMON  TAV,    TF,     TIT1(20), TZERO, TS                           00500120
      COMMON  XLAMB,  XN1,    XN2,    XN3,    XNU,    XNU1                  00500130
      COMMON  XSTAP,  XSTARD, XSTPD,  XSTPF,  XNUP,   FTAP                  00500140
      COMMON  PMW,    IPLT,   GAM,    DEL,    XNUU,   WAP                   00500150
      COMMON  PR1,    PR2,    PR3,    PR4,    PR6,    PR7                   00500160
      COMMON PR8                                                            00500170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)                   00500180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                       00500190
      COMMON CZERO,SIGC,CRIT,QSOLID                                         00500200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                                 00500210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                          00500220
      COMMON C25(20),NJOB,IJX                                               00500230
      COMMON SII(20),QLIQ                                                   00500240
      COMMON INI,M1                                                         00500250
      COMMON QAL                                                            00500260
C                                                                           00500270
      DIMENSION PTA(30),BRA(30),BETI(30),CTL(30),DELL(30),GAMM(30)          00500280
      DIMENSION SI(30),SIC(30)                                              00500290
      GO TO (1,2), I                                                        00500300
1     DELL(K)=DEL                                                           00500310
      GAMM(K)=GAM                                                           00500320
      SI(K)=SIGC                                                            00500330
      SIC(K)=SIGSC                                                          00500340
      RETURN                                                                00500350
2     CONTINUE                                                              00500360
```

CARD NO **** CONTENTS ****

```
           WRITE(6,3)                                                          00500370
           DO 4 J=1,KMAX                                                       00500380
           WRITE(6,5)PTA(J),BRA(J),BETI(J),DELL(J),SI(J),SIC(J),GAMM(J),       00500390
          *         CTL(J)                                                     00500400
 4         CONTINUE                                                            00500410
           RETURN                                                              00500420
         3 FORMAT(2X'PT,PSIA  BF, IN/SEC  BETAF       DELTA  SIGC    SIGSC'    00500430
          *       2X'GAMMA'5X'CRIT'//)                                         00500440
         5 FORMAT(F9.1,F9.4,F11.4,F11.3,3F7.3,F9.3)                            00500450
           END                                                                 00500460
           SUBROUTINE OXID1(N)                                                 00600010
 C                                                                             00600020
           COMMON  A1,     A2,      AF,       AFH,    ALFA,    RHAL            00600030
           COMMON  AOX,    BESS,    BETAF,  BSOR,   C3P                        00600040
           COMMON  C4P,    CIGN,    CON1,     CSUBP,  DELDI,   DZERO           00600050
           COMMON  FF,     EOX,     ETA,      GAMMA,  GMW,     HON             00600060
           COMMON  HDP,    IJIM,    IPLOT,    K,      KAP1,    KAP2            00600070
           COMMON  KPF,    EPS,    MOX,      MT,     NP1,     P                00600080
           COMMON  POWD,   POWIGN,  PSTART,   PSTOP,  QAP,     QFF             00600090
           COMMON  QFUEL,  QL,      QPF,      R,      RAP,     RF              00600100
           COMMON  RHOF,   RHOP,    RHOX,     RON,    SOX,     TAP             00600110
           COMMON  TAV,    TF,      TIT1(20), TZERO,  TS                       00600120
           COMMON  XLAMB,  XN1,     XN2,      XN3,    XNU,     XNU1            00600130
           COMMON  XSTAP,  XSTARD,  XSTPD,    XSTPF,  XNUP,    ETAP            00600140
           COMMON  PMW,    IPLT,    GAM,      DEL,    XNUU,    WAP             00600150
           COMMON  PR1,    PR2,     PR3,      PR4,    PR6,     PR7             00600160
           COMMON PR8                                                          00600170
           COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)                 00600180
           COMMON NN,RHOPI,XNUSC,RON1,RONN                                     00600190
           COMMON CZERO,SIGC,CRIT,OSOLID                                       00600200
           COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                               00600210
           COMMON AFH1,ME,XSPD,XSAP,ISI                                        00600220
           COMMON C25(20),NJOB,IJX                                             00600230
           COMMON SII(20),QLIQ                                                 00600240
           COMMON INI,M1                                                       00600250
           COMMON QAL                                                          00600260
 C                                                                             00600270
           DO 2 J=1,NN                                                         00600280
           DMA=ALOG(DMAX(J))                                                   00600290
           DMI=ALOG(DMIN(J))                                                   00600300
           SLP(J)=(DMA-DMI)                                                    00600310
           DZE=SLP(J)*.5+DMI                                                   00600320
           DZERO1(J)=EXP(DZE)                                                  00600330
 2         CONTINUE                                                            00600340
           CRIT=10.0                                                           00600350
           RETURN                                                              00600360
           END                                                                 00600370
           SUBROUTINE CONCAL                                                   00700010
 C                                                                             00700020
           COMMON  A1,     A2,      AF,       AFH,    ALFA,    RHAL            00700030
```

```
      COMMON  AOX,    BESS,     BETAF, BSQF,    C3P
      COMMON  C4P,    CIGN,     CON1,           CSUBP, DELDI,  DZERO
      COMMON  EF,     EOX,      ETA,            GAMMA, GMW,    HON
      COMMON  HDP,    IJIM,     IPLOT,          K,     KAP1,   KAP2
      COMMON  KPF,    EPS,     MOX,            MT,    NP1,     P
      COMMON  POWD,   POWIGN,   PSTART,         PSTCP, QAP,    QFF
      COMMON  QFUEL,  QL,       QPF,            R,     RAP,    RF
      COMMON  RHOF,   RHOP,     RHOX,           RON,   SOX,    TAP
      COMMON  TAV,    TF,       TIT1(20),       TZERO, TS
      COMMON  XLAMB,  XN1,      XN2,            XN3,   XNU,    XNU1
      COMMON  XSTAP,  XSTARD,   XSTPD,          XSTPF, XNUP,   ETAP
      COMMON  PMW,    IPLT,     GAM,            DEL,   XNUU,   WAP
      COMMON  PR1,    PR2,      PR3,            PR4,   PR6,    PR7
      COMMON  PR8
      COMMON  DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)
      COMMON  NN,RHOPI,XNUSC,RON1,RONN
      COMMON  CZERO,SIGC,CRIT,QSOLID
      COMMON  SIGSC,IX,LLL,RN,AH,C10,C15,C20
      COMMON  AFH1,MF,XSPD,XSAP,ISI
      COMMON  C25(20),NJOB,IJX
      COMMON  SII(20),QLIQ
      COMMON  INI,M1
      COMMON  QAL
C
      REAL KAP1,KAP2,KPF,MOX,MT
      DIMENSION FAC(10)
      J=INI
    1 IF (J)2,2,15
    2 FAC(1)=1.
      FAC(2)=1.36055
      FAC(3)=1.7007
      FAC(4)=2.04082
      FAC(5)=2.7211
      FAC(6)=3.4014
      FAC(7)=4.76191
      FAC(8)=6.80273
      FAC(9)=8.16327
      FAC(10)=10.20409
      JJ=0
      I=1
   15 IF (JJ-1)16,20,20
   16 XMULT=PSTART
      JJ=1
      I=8
   20 IF(IJIM.EQ.0)GO TO 22
      I=I-3
      K=K-2
      IJIM=0
   22 IF(I-11)50,21,21
   21 XMULT=XMULT*10.
      I=2
   50 P=XMULT*FAC(I)
      I=I+1
      LLL=1
      RETURN
      END
```

```
      SUBROUTINE CONVR                                                  00800010
      EXTERNAL SURFAC                                                   00800020
C                                                                       00800030
      COMMON   A1,     A2,      AF,      AFH,     ALFA,    RHAL        00800040
      COMMON   AOX,    BESS,    BETAF,   BSOP,    C3P                 00800050
      COMMON   C4P,    CIGN,    CONI,    CSURP,   DELDI,   DZERO       00800060
      COMMON   EE,     EOX,     ETA,     GAMMA,   GMW,     HON         00800070
      COMMON   HOP,    IJIM,    IPLOT,   K,       KAP1,    KAP2        00800080
      COMMON   KPE,    EPS,     MOX,     MT,      NP1,     P           00800090
      COMMON   POWD,   POWIGN,  PSTART,  PSTOP,   QAP,     QFF         00800100
      COMMON   QFUEL,  QL,      QPE,     R,       RAP,     RE          00800110
      COMMON   RHOE,   RHOP,    RHOX,    RON,     SOX,     TAP         00800120
      COMMON   TAV,    TF,      TIT1(20),TZERO,   TS                  00800130
      COMMON   XLAMB,  XN1,     XN2,     XN3,     XNU,     XNU1        00800140
      COMMON   XSTAP,  XSTARD,  XSTPD,   XSTPE,   XNUP,    ETAP        00800150
      COMMON   PMW,    IPLT,    GAM,     DEL,     XNUU,    WAP         00800160
      COMMON   PR1,    PR2,     PR3,     PR4,     PR6,     PR7         00800170
      COMMON PR8                                                        00800180
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)               00800190
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                   00800200
      COMMON CZERO,SIGC,CRIT,QSOLID                                     00800210
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                             00800220
      COMMON AFH1,ME,XSPD,XSAP,ISI                                      00800230
      COMMON C25(20),NJOB,IJX                                           00800240
      COMMON SII(20),QLIQ                                               00800250
      COMMON INI,M1                                                     00800260
      COMMON QAL                                                        00800270
C                                                                       00800280
      DIMENSION ARLST(2)                                                00800290
      I7=0                                                              00800300
      I8=0                                                              00800310
      NE=1                                                              00800320
      XSPD=XSTPD                                                        00800330
      XSAP=XSTAP                                                        00800340
      ARLST(1)=CRIT                                                     00800350
1     ACRIT=CRIT-ROOT(SURFAC,ARLST)                                     00800360
      IF(ABS(1.-ACRIT/CRIT)-.01)2,2,3                                   00800370
3     IF(CRIT-ACRIT)4,2,5                                               00800380
5     I7=1                                                              00800390
      XLOW=ACRIT                                                        00800400
      GO TO 6                                                           00800410
4     I8=1                                                              00800420
      XUP=AMIN1(ACRIT,50.)                                              00800430
6     IF(I7+I8-2)7,8,8                                                  00800440
7     ARLST(1)=ACRIT                                                    00800450
C     WRITE(6,100) NE , CRIT                                            00800460
C 100 FORMAT(10X,I5,5X,E15.8)                                           00800470
      NE=NE+1                                                           00800480
      GO TO 1                                                           00800490
8     ANS=0.02                                                          00800500
```

```
CARD NO       ****                          CONTENTS                                   ****

                    N=15                                                            00800510
              C     WRITE(6,110) CRIT, XUP , XLOW                                   00800520
              C 110 FORMAT(10X,5E16.8)                                              00800530
                    CRIT=CONVR3(SURFAC,ARLST,XUP,XLOW,ANS,N)                        00800540
              C     WRITE(6,120) CRIT                                               00800550
              C 120 FORMAT(10X'CRIT= ',E15.9)                                       00800560
              2     CONTINUE                                                        00800570
                    RETURN                                                          00800580
                    END                                                             00800590
                    FUNCTION ROB(XNAME,ARLST)                                       00900010
                    EXTERNAL XNAME                                                  00900020
                    DIMENSION ARLST(2)                                              00900030
                    ROB=XNAME(ARLST)                                                00900040
                    RETURN                                                          00900050
                    END                                                             00900060
                    FUNCTION SURFAC(ARLST)                                          01000010
              C                                                                     01000020
                    COMMON  A1,     A2,      AF,         AFH,    ALFA,   RHAL       01000030
                    COMMON  AOX,    BESS,    BETAF, BSQR,   C3P                     01000040
                    COMMON  C4P,    CIGN,    CON1,       CSUBP,  DFLDI,  DZERO      01000050
                    COMMON  FF,     FOX,     FTA,        GAMMA,  GMW,    HDN        01000060
                    COMMON  HDP,    IJIM,    IPLOT,      K,      KAP1,   KAP2       01000070
                    COMMON  KPF,    FPS,    MOX,        MT,     NP1,    P           01000080
                    COMMON  POWD,   POWIGN,  PSTART,     PSTOP,  QAP,    QFF        01000090
                    COMMON  QFUEL,  QL,      QPF,        R,      RAP,    RF         01000100
                    COMMON  RHOF,   RHOP,    RHOX,       RON,    SOX,    TAP        01000110
                    COMMON  TAV,    TF,      TIT1(20),   TZERO,  TS                 01000120
                    COMMON  XLAMB,  XN1,     XN2,        XN3,    XNU,    XNU1       01000130
                    COMMON  XSTAP,  XSTARD,  XSTPD,      XSTPF,  XNUP,   FTAP       01000140
                    COMMON  PMW,    IPLT,    GAM,        DEL,    XNUU,   WAP        01000150
                    COMMON  PR1,    PR2,     PR3,        PR4,    PR6,    PR7        01000160
                    COMMON PR8                                                      01000170
                    COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)             01000180
                    COMMON NN,RHOPI,XNUSC,RON1,RONN                                 01000190
                    COMMON CZERO,SIGC,CRIT,QSOLID                                   01000200
                    COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                           01000210
                    COMMON AFH1,ME,XSPD,XSAP,ISI                                    01000220
                    COMMON C25(20),NJOB,IJX                                         01000230
                    COMMON SII(20),QLIQ                                             01000240
                    COMMON INI,M1                                                   01000250
                    COMMON QAL                                                      01000260
              C                                                                     01000270
                    DIMENSION ARLST(2)                                              01000280
                    CRIT=ARLST(1)                                                   01000290
                    CALL OXID(2)                                                    01000300
                    CALL STAMP1                                                     01000310
                    ACRIT=CRTL(TS,R)                                                01000320
                    SURFAC=APLST(1)-ACRIT                                           01000330
              C     WRITE(6,101) ACRIT                                              01000340
              C 101 FORMAT(10X'CRIT = ',E15.8)                                      01000350
```

```
      RETURN                                                                    01000360
      END                                                                       01000370
      FUNCTION CONVR3 (XNAME,ARGLST,XUP,XLOW,ANS,N)                             01100010
      EXTERNAL XNAME                                                            01100020
      DIMENSION ARGLST(20)                                                      01100030
      BOT=XLOW                                                                  01100040
      XINC=(XUP-XLOW)*0.5                                                       01100050
      TOP=XLOW+XINC                                                             01100060
      IVAL=N                                                                    01100070
      ARGLST(1)=BOT                                                             01100080
      ABOT=XNAME(ARGLST)                                                        01100090
      ARGLST(1)=XUP                                                             01100100
      ATOP=XNAME(ARGLST)                                                        01100110
      IF ((ATOP-ANS)*(ABOT-ANS))30,30,31                                        01100120
31    IF (ABS(ATOP-ANS)-ABS(ABOT-ANS))32,32,33                                  01100130
32    CONVR3=XUP                                                                01100140
      GO TO 99                                                                  01100150
33    CONVR3=XLOW                                                               01100160
      GO TO 99                                                                  01100170
30    ARGLST(1)=TOP                                                             01100180
      ATOP=XNAME(ARGLST)                                                        01100190
50    CONTINUE                                                                  01100200
      IF ((ATOP-ANS)*(ABOT-ANS))1,40,2                                          01100210
1     XINC=XINC*.5                                                              01100220
      TOP=BOT+XINC                                                              01100230
      IVAL=IVAL-1                                                               01100240
      IF (IVAL)12,12,11                                                         01100250
12    CONVR3=TOP                                                                01100260
      GO TO 99                                                                  01100270
11    ARGLST(1)=TOP                                                             01100280
      ATOP=XNAME(ARGLST)                                                        01100290
      GO TO 50                                                                  01100300
2     XINC=XINC*0.5                                                             01100310
      BOT=TOP                                                                   01100320
      TOP=BOT+XINC                                                              01100330
      ABOT=ATOP                                                                 01100340
      IVAL=IVAL-1                                                               01100350
      IF (IVAL)22,22,21                                                         01100360
22    CONVR3=TOP                                                                01100370
      GO TO 99                                                                  01100380
21    ARGLST(1)=TOP                                                             01100390
      ATOP=XNAME(ARGLST)                                                        01100400
      GO TO 50                                                                  01100410
40    IF (ATOP-ANS)42,41,42                                                     01100420
41    CONVR3=TOP                                                                01100430
      GO TO 99                                                                  01100440
42    CONVR3=BOT                                                                01100450
99    CONTINUE                                                                  01100460
      RETURN                                                                    01100470
      END                                                                       01100480
      FUNCTION CRTL(TE,RE)                                                      01200010
C                                                                               01200020
      COMMON  A1,     A2,     AF,     AFH,    ALFA,   PHAL                      01200030
      COMMON  AOX,    BESS,   BETAF,  BSQR,   C3P                               01200040
      COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO                     01200050
      COMMON  EF,     EOX,    ETA,    GAMMA,  GMW,    HON                       01200060
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```
      COMMON  HDP,    IJIM,     IPLOT,      K,      KAP1,    KAP2          01200070
      COMMON  KPF,    EPS,     MOX,        MT,     NP1,     P             01200080
      COMMON  POWD,   POWIGN,   PSTART,     PSTOP,  QAP,     QFF           01200090
      COMMON  QFUEL,  QL,       QPF,        R,      RAP,     RF            01200100
      COMMON  RHOF,   RHOP,     RHOX,       RON,    SOX,     TAP           01200110
      COMMON  TAV,    TF,       TIT1(20),   TZERO,  TS                    01200120
      COMMON  XLAMB,  XN1,      XN2,        XN3,    XNU,     XNU1          01200130
      COMMON  XSTAP,  XSTARD,   XSTPD,      XSTPF,  XNUP,    ETAP          01200140
      COMMON  PMW,    IPLT,     GAM,        DEL,    XNUU,    WAP           01200150
      COMMON  PR1,    PR2,      PR3,        PR4,    PR6,     PR7           01200160
      COMMON PR8                                                          01200170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)                 01200180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                     01200190
      COMMON CZERO,SIGC,CRIT,QSOLID                                       01200200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                               01200210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                        01200220
      COMMON C25(20),NJOB,IJX                                             01200230
      COMMON SII(20),QLIQ                                                 01200240
      COMMON INI,MI                                                       01200250
      COMMON QAL                                                          01200260
C                                                                         01200270
      DELL=TE-TZERO                                                       01200280
      RR=DELL*RE/.0011                                                    01200290
      IF(TE.GT.723.)GO TO 5                                               01200300
      CRTL=0.0                                                            01200310
      SIGSC=1.0                                                           01200320
      RETURN                                                              01200330
5     CONTINUE                                                            01200340
      DELLL=TE-673.                                                       01200350
      CRTL=DELLL/RR*10000.                                                01200360
      RETURN                                                              01200370
      END                                                                 01200380
      SUBROUTINE OXID (N)                                                 01300010
C                                                                         01300020
      COMMON  A,      A2,       AF,         AFH,    ALFA,    RHAL          01300030
      COMMON  AGX,    BESS,     BETAF, BSQR,    C3P                       01300040
      COMMON  C4P,    CIGN,     CON1,       CSUBP,  DELDI,   DZERO         01300050
      COMMON  EF,     EOX,      ETA,        GAMMA,  GMW,     HDN           01300060
      COMMON  HDP,    IJIM,     IPLOT,      K,      KAP1,    KAP2          01300070
      COMMON  KPF,    EPS,     MOX,        MT,     NP1,     P             01300080
      COMMON  POWD,   POWIGN,   PSTART,     PSTOP,  QAP,     QFF           01300090
      COMMON  QFUEL,  QL,       QPF,        R,      RAP,     RF            01300100
      COMMON  RHOF,   RHOP,     RHOX,       RON,    SOX,     TAP           01300110
      COMMON  TAV,    TF,       TIT1(20),   TZERO,  TS                    01300120
      COMMON  XLAMB,  XN1,      XN2,        XN3,    XNU,     XNU1          01300130
      COMMON  XSTAP,  XSTARD,   XSTPD,      XSTPF,  XNUP,    ETAP          01300140
      COMMON  PMW,    IPLT,     GAM,        DEL,    XNUU,    WAP           01300150
      COMMON  PR1,    PR2,      PR3,        PR4,    PR6,     PR7           01300160
      COMMON PRR                                                          01300170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)                 01300180
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CARD NO	****	CONTENTS	****
778		COMMON NN,RHOPI,XNUSC,RON1,RONN	01300190
779		COMMON CZERO,SIGC,CRIT,QSOLID	01300200
780		COMMON SIGSC,IX,LLL,PN,AH,C10,C15,C20	01300210
781		COMMON AFHI,MF,XSPD,XSAP,ISI	01300220
782		COMMON C25(20),NJOB,IJX	01300230
783		COMMON SII(20),QLIQ	01300240
784		COMMON INI,MI	01300250
785		COMMON QAL	01300260
786	C		01300270
787		DIMENSION A(20),CC(20)	01300280
788		DIMENSION SI(20)	01300290
789		DO 3 J=1,NN	01300300
790		SI(J)=0.0	01300310
791		A(J)=0.0	01300320
792		CC(J)=0.0	01300330
793	3	CONTINUE	01300340
794		RON=0.0	01300350
795		DZERO=0.0	01300360
796		SIGC=0.0	01300370
797		SIGSC=0.0	01300380
798		DO 10 J=1,NN	01300390
799		NM=J	01300400
800		IF(CRIT.LE.0.01) GO TO 10	01300410
801		IF(DMIN(J).LE.CRIT-0.01)GO TO 16	01300420
802	10	CONTINUE	01300430
803		DO 15 J=1,NN	01300440
804		B=DMIN(J)	01300450
805		D=DMAX(J)	01300460
806		CALL PART(B,D)	01300470
807		RON=RON+SIG(J)*RON1	01300480
808	15	DZERO=DZERO+SIG(J)*DZERO1(J)	01300490
809		SIGC=0.0	01300500
810		SIGSC=1.0	01300510
811		RETURN	01300520
812	16	CONTINUE	01300530
813		MMM=NM-1	01300540
814	20	J=NM	01300550
815	31	IF(DMAX(J).GT.CRIT)GO TO 25	01300560
816		SIGC=SIGC+SIG(J)	01300570
817	C	WRITE(6,100) SIGC	01300580
818	C 100	FORMAT(10X,'ONE',E16.8)	01300590
819		J=J+1	01300600
820		IF(J.LE.NN)GO TO 31	01300610
821		GO TO 28	01300620
822	25	CR=ALOG(CRIT)	01300630
823		DMI=ALOG(DMIN(J))	01300640
824		DMA=ALOG(DMAX(J))	01300650
825		DZE=ALOG(DZERO1(J))	01300660
826		A(J)=(CR-DMI)/SLP(J)	01300670
827	C	WRITE(6,101) SLP(J), A(J)	01300680

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      C 101 FORMAT(10X,'SLP= ',F16.8,'    A(J)= ',F16.8)                        01300690
            SIGC=SIGC+A(J)*SIG(J)                                               01300700
            C=SLP(J)*((1.-A(J))/2.0+A(J))+DMI                                   01300710
            CC(J)=EXP(C)                                                        01300720
      C     WRITE(6,102) CC(J), SIGC , SIGSC                                    01300730
      C 102 FORMAT(3E16.7)                                                      01300740
            J=J+1                                                               01300750
            IF(J.LE.NN)GO TO 31                                                 01300760
            J=NM                                                                01300770
            SIGSC=1.-SIGC                                                       01300780
      C     WRITE(6,103) SIGSC                                                  01300790
      C 103 FORMAT(10X'SIGSC= ',E16.7)                                          01300800
      45    SI(J)=SIG(J)*(1.-A(J))/SIGSC                                        01300810
            B=DMAX(J)                                                           01300820
            CALL PART(CRIT,B)                                                   01300830
            RON=RON+SI(J)*RON1                                                  01300840
            SII(J)=SI(J)                                                        01300850
            DZERO=DZERO+SI(J)*CC(J)                                             01300860
            J=J+1                                                               01300870
            IF(J.LE.NN) GO TO 45                                                01300880
            GO TO 30                                                            01300890
      28    CONTINUE                                                            01300900
            SIGSC=1.-SIGC                                                       01300910
      30    DO 40 J=1,MMM                                                       01300920
            SI(J)=SIG(J)/(1.-SIGC)                                              01300930
            B=DMIN(J)                                                           01300940
            D=DMAX(J)                                                           01300950
            CALL PART(B,D)                                                      01300960
            RON=RON+SI(J)*RON1                                                  01300970
            SII(J)=SI(J)                                                        01300980
      40    DZERO=DZERO+SI(J)*DZERO1(J)                                         01300990
      44    CONTINUE                                                            01301000
            RETURN                                                              01301010
            END                                                                 01301020
            SUBROUTINE PART(DMI,DMA)                                            01400010
      C                                                                         01400020
            COMMON  A1,     A2,       AF,          AFH,    ALFA,    RHAL      01400030
            COMMON  AOX,    BESS,     BETAF, BSQR,    C3P                     01400040
            COMMON  C4P,    CIGN,     CON1,        CSUBP, DELDI,   DZERO     01400050
            COMMON  EF,     EOX,      ETA,         GAMMA, GMW,     HDN       01400060
            COMMON  HDP,    IJIM,     IPLOT,       K,     KAP1,    KAP2      01400070
            COMMON  KPF,    EPS,    MOX,         MT,    NP1,     P          01400080
            COMMON  POWD,   POWIGN,   PSTART,      PSTOP, QAP,     QFF       01400090
            COMMON  QFUEL,  QL,       QPF,         R,     RAP,     RF        01400100
            COMMON  RHOF,   RHOP,     RHOX,        RON,   SOX,     TAP       01400110
            COMMON  TAV,    TF,       TIT1(20),    TZERO, TS                01400120
            COMMON  XLAMB,  XN1,      XN2,         XN3,   XNU,     XNU1      01400130
            COMMON  XSTAP,  XSTARD,   XSTPD,       XSTPF, XNUP,    ETAP      01400140
            COMMON  PMW,    IPLT,     GAM,         DEL,   XNUU,    WAP       01400150
            COMMON  PR1,    PR2,      PR3,         PR4,   PR6,     PR7       01400160
            COMMON PR8                                                        01400170
            COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)               01400180
            COMMON NN,RHOPI,XNUSC,RON1,RONN                                   01400190
            COMMON CZERO,SIGC,CRIT,QSOLID                                     01400200
            COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                             01400210
            COMMON AFH1,ME,XSPD,XSAP,ISI                                      01400220
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      COMMON C25(20),NJOB,IJX                                           01400230
      COMMON SII(20),QLIQ                                               01400240
      COMMON INI,MI                                                     01400250
      COMMON QAL                                                        01400260
C                                                                       01400270
      PAR=DMI                                                           01400280
      RON1=(DMI*0.0001)**POWD                                           01400290
      RON1=RON1/P**POWIGN                                               01400300
      DELZ=(DMA-DMI)/10.                                                01400310
      DO 10 J=1,10                                                      01400320
      PAR=PAR+DELZ                                                      01400330
      DZE=(PAR*0.0001)**POWD                                            01400340
      DZE=DZE/P**POWIGN                                                 01400350
      RON1=RON1+DZE                                                     01400360
10    CONTINUE                                                          01400370
      RON1=RON1/11.                                                     01400380
      RETURN                                                            01400390
      END                                                               01400400
      SUBROUTINE STAMP1                                                 01500010
      EXTERNAL DON1                                                     01500020
C                                                                       01500030
      COMMON  A1,     A2,     AF,     AFH,    ALFA,   AHAL            01500040
      COMMON  AOX,    BESS,   BETAF,  BSQR,   C3P                     01500050
      COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO           01500060
      COMMON  FF,     FOX,    FTA,    GAMMA,  GMW,    HON             01500070
      COMMON  HOP,    IJIM,   IPLOT,  K,      KAP1,   KAP2            01500080
      COMMON  KPF,    EPS,    MOX,    MT,     NP1,    P               01500090
      COMMON  POWD,   POWIGN, PSTART, PSTOP,  QAP,    QFF             01500100
      COMMON  QFUEL,  QL,     QPF,    R,      RAP,    RF              01500110
      COMMON  RHOF,   RHOP,   RHOX,   RON,    SOX,    TAP             01500120
      COMMON  TAV,    TF,     TIT1(20),TZERO, TS                      01500130
      COMMON  XLAMB,  XN1,    XN2,    XN3,    XNU,    XNU1            01500140
      COMMON  XSTAP,  XSTARO, XSTPO,  XSTPF,  XNUP,   ETAP            01500150
      COMMON  PMW,    IPLT,   GAM,    DEL,    XNUU,   WAP             01500160
      COMMON  PR1,    PR2,    PR3,    PR4,    PR6,    PR7             01500170
      COMMON PR8                                                        01500180
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)               01500190
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                   01500200
      COMMON CZERO,SIGC,CRIT,QSOLID                                     01500210
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                             01500220
      COMMON AFH1,ME,XSPO,XSAP,ISI                                      01500230
      COMMON C25(20),NJOB,IJX                                           01500240
      COMMON SII(20),QLIQ                                               01500250
      COMMON INI,MI                                                     01500260
      COMMON QAL                                                        01500270
C                                                                       01500280
      DIMENSION AN(4)                                                   01500290
      DIMENSION ARGLST(20)                                              01500300
      REAL KAP1,KAP2,KPF,MOX,MT                                         01500310
      REAL MOX70                                                        01500320
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CARD NO   ****                        CONTENTS                                  ****

934             REAL*8 ARG,AN                                                   01500330
935             GAM=ALFA*(1.-SIGC)                                              01500340
936             WF=(1.-EPS-ALFA)/(1.-EPS-GAM)                                   01500350
937             IF(WF.GT.1.0)WF=1.0                                             01500360
938             XNUU=1./(1.+RHOF*(1.-WF)/(WF*RHOX))                             01500370
939             IF(XNUU.GT.1.0)XNUU=1.0                                         01500380
940             RHOPI=RHOF*XNUU/WF                                              01500390
941             IF(RHOPI.LT.RHOF)RHOPI=RHOF                                     01500400
942             XNUSC=1./(1.+RHOX*(1.-EPS-GAM)/(GAM*RHOPI))                     01500410
943             IF(XNUSC.GT.1.)XNUSC=1.0                                        01500420
944             DEL=1.11*ALFA*SIGC/(1.-EPS-GAM)                                 01500430
945       10    CONTINUE                                                        01500440
946             RHOP=RHOX*XNU/ALFA                                              01500450
947             DELD=1+EPS*RHOX/(GAM*RHAL)+RHOX*(1.-GAM-EPS)/(RHOPI*GAM)        01500460
948             IF(DELD.LT.1.0)DELD=1.0                                         01500470
949             DELDI=(3.141592/6.*DELD)**(1./3.)-SQRT(2./3.)                   01500480
950             BSQR=DZERO**2/6.*(1.+SQRT(1.5)*DELDI)**2*1.0E-08                01500490
951             CON1=1./(1.+SQRT(1.5)*DELDI)                                    01500500
952             C=XNUP-(1.+XNUP)*CON1*CON1                                      01500510
953             C=C/(2.*(1.+XNUP)*CON1)                                         01500520
954             C10=C                                                           01500530
955             C11=XNU1-(1.+XNU1)*CON1*CON1                                    01500540
956             C11=C11/(2.*(1.+XNU1)*CON1)                                     01500550
957             ARG=3.83*CON1                                                   01500560
958             IBB=1                                                           01500570
959             CALL BESSEL(0.D0,ARG,AN)                                        01500580
960             BESS=AN(3)                                                      01500590
961             DUM1 = CON1*BESS*(1.+XNU1)/(XNU1-(1.+XNU1)*CON1**2)             01500595
962             IF(DUM1)20,22,24                                                01500600
963       20    ETA = ALOG(-1.293*DUM1)                                         01500605
964             GO TO 26                                                        01500610
965       22    ETA = 0.0                                                       01500615
966             GO TO 26                                                        01500620
967       24    ETA = ALOG(3.215*DUM1)                                          01500625
968       26    DUM1 = CON1*BESS*(1.+XNUP)/(XNUP-(1.+XNUP)*CON1**2)             01500630
969             IF(DUM1)30,32,34                                                01500635
970       30    ETAP= ALOG(-1.293*DUM1)                                         01500640
971             GO TO 36                                                        01500645
972       32    ETAP= 0.0                                                       01500650
973             GO TO 36                                                        01500655
974       34    ETAP= ALOG(3.215*DUM1)                                          01500660
975             IBB=2                                                           01500670
976       36    CONTINUE                                                        01500680
977             CON2=GAMMA*TAV**0.75/82.06*GMW                                  01500690
978             C3=2.*CON2*ETA*AFH1                                             01500700
979             C4=(7.66*CON2)**2/BSQR                                          01500710
980             XNC=XN2                                                         01500720
981             RATC=KAP1                                                       01500730
982             MT=RHOP*F                                                       01500740
983             XMT=0.                                                          01500750
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      51    I7=0                                                          01500760
            I8=0                                                          01500770
            ARGLST(1)=TS                                                  01500780
            ARGLST(3)=C3                                                  01500790
            ARGLST(4)=C4                                                  01500800
            ARGLST(5)=RATC                                                01500810
            ARGLST(6)=XNC                                                 01500820
            ARGLST(7)=C                                                   01500830
            ARGLST(8)=CON2                                                01500840
            ARGLST(9)=C11                                                 01500850
            ARGLST(10)=IBB                                                01500860
      80    XTS=TS-BOB(DON1,ARGLST)                                       01500870
            IF(ABS(1.-XTS/TS)-.001)60,60,61                               01500880
      61    IF (TS-XTS)85,60,85                                           01500890
      85    I7=1                                                          01500900
            XLOW=XTS                                                      01500910
            GO TO 87                                                      01500920
      86    I8=1                                                          01500930
            XUP=AMIN1(XTS,1400.)                                          01500940
      87    IF (I7+I8-2)88,89,89                                          01500950
      88    ARGLST(1)=XTS                                                 01500960
            GO TO 80                                                      01500970
      89    ANS=0.0001                                                    01500980
            N=15                                                          01500990
            XTS=CONVR2(DON1,ARGLST,XUP,XLOW,ANS,N)                        01501000
      60    CONTINUE                                                      01501010
      62    R=MT/RHOP                                                     01501020
C           WRITE(6,100)                                                  01501030
C 100 FORMAT(10X'TWO')                                                    01501040
            RETURN                                                        01501050
            END                                                           01501060
            SUBROUTINE BESSEL(X,Y,ANS)                                    01600010
            DIMENSION ANS(4)                                              01600020
            REAL*8 X,Y,ANS,Z,FZERO,THZERO,FONE,THONE                      01600030
            IF(X-3.D0)2,2,4                                               01600040
      2     Z=X*X/9.                                                      01600050
            IF(X)20,20,30                                                 01600060
      20    ANS(1)=1.                                                     01600070
            ANS(2)=1.                                                     01600080
            GO TO 6                                                       01600090
      30    CONTINUE                                                      01600100
            ANS(1)=(((((.00021*Z-.0039444)*Z+.0444479)*Z-.3163866)*       01600110
           &Z+1.2656208)*Z-2.2499997)*Z+1.                                01600120
            ANS(2)=.63662031*DLOG(.5*X)*ANS(1)+(((((-.00024846*Z+         01600130
           &.00427916)*Z-.04261214)*Z+.25300117)*Z-.74350384)*Z+.60       01600140
           &559366)*Z+.36746691                                           01600150
            GO TO 6                                                       01600160
      4     Z=3./X                                                        01600170
            FZERO=(((((.00014476*Z-.00072805)*Z+.00137237)*Z-.0000        01600180
           &9512)*Z-.0055274)*Z-.77E-6)*Z+.79788456                       01600190
            THZERO=X+(((((.00013558*Z-.00029333)*Z-.00054125)*Z+.00       01600200
           &262573)*Z-.00003954)*Z-.04166397)*Z-.78539816                 01600210
            ANS(1)=FZERO*DCOS(THZERO)/DSQRT(X)                            01600220
            ANS(2)=FZERO*DSIN(THZERO)/DSQRT(X)                            01600230
      6     IF(Y-3.D0)8,8,10                                              01600240
      8     Z=Y*Y/9.                                                      01600250
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1040              IF(Y)40,40,50                                                  01600260
1041        40    ANS(3)=0.                                                      01600270
1042              ANS(4)=0.                                                      01600280
1043              GO TO 80                                                       01600290
1044        50    CONTINUE                                                       01600300
1045              ANS(3)=((((((.00001109*Z-.0003176)*Z+.00443319)*Z-.0395        01600310
1046             &42289)*Z+.21093573)*Z-.5649985)*Z+.5)*Y                        01600320
1047              ANS(4)=(.63662031*Y*DLOG(.5*Y)*ANS(3)+(((((.0027873*Z-         01600330
1048             &.0400976)*Z+.3123951)*Z-1.3164827)*Z+2.1682709)*Z+.2212        01600340
1049             &0911)*Z-.6366198)/Y                                            01600350
1050        80    RETURN                                                         01600360
1051        10    Z=3./Y                                                         01600370
1052              FONE=(((((-.0020033*Z+.00113653)*Z-.00249511)*Z+.00017         01600380
1053             &105)*Z+.01553667)*Z+1.56E-6)*Z+.79788456                       01600390
1054              THONE=Y+(((((-.00029166*Z+.00079824)*Z+.00074348)*Z-.00        01600400
1055             &637879)*Z+.00005650)*Z+.12499512)*Z-2.3561945                  01600410
1056              ANS(3)=FONE*DCOS(THONE)/DSQRT(Y)                               01600420
1057              ANS(4)=FONE*DSIN(THONE)/DSQRT(Y)                               01600430
1058              RETURN                                                         01600440
1059              END                                                            01600450
1060              FUNCTION BOB(XNAME,ARGLST)                                     01700010
1061              EXTERNAL XNAME                                                 01700020
1062              DIMENSION ARGLST(20)                                           01700030
1063              BOB=XNAME(ARGLST)                                              01700040
1064              RETURN                                                         01700050
1065              END                                                            01700060
1066              FUNCTION CONVR2 (XNAME,ARGLST,XUP.XLOW,ANS,N)                  01800010
1067              EXTERNAL XNAME                                                 01800020
1068              DIMENSION ARGLST(20)                                           01800030
1069              BOT=XLOW                                                       01800040
1070              XINC=(XUP-XLOW)*0.5                                            01800050
1071              TOP=XLOW+XINC                                                  01800060
1072              IVAL=N                                                         01800070
1073              ARGLST(1)=BOT                                                  01800080
1074              ABOT=XNAME(ARGLST)                                             01800090
1075              ARGLST(1)=XUP                                                  01800100
1076              ATOP=XNAME(ARGLST)                                             01800110
1077              IF ((ATOP-ANS)*(ABOT-ANS))30,30,31                             01800120
1078        31    IF (ABS(ATOP-ANS)-ABS(ABOT-ANS))32,32,33                       01800130
1079        32    CONVR2=XUP                                                     01800140
1080              GO TO 99                                                       01800150
1081        33    CONVR2=XLOW                                                    01800160
1082              GO TO 99                                                       01800170
1083        30    ARGLST(1)=TOP                                                  01800180
1084              ATOP=XNAME(ARGLST)                                             01800190
1085        50    CONTINUE                                                       01800200
1086              IF ((ATOP-ANS)*(ABOT-ANS))1,40,2                               01800210
1087        1     XINC=XINC*.5                                                   01800220
1088              TOP=BOT+XINC                                                   01800230
1089              IVAL=IVAL-1                                                    01800240
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      IF (IVAL)12,12,11                                                 01800250
12    CONVR2=TOP                                                        01800260
      GO TO 99                                                          01800270
11    ARGLST(1)=TOP                                                     01800280
      ATOP=XNAME(ARGLST)                                                01800290
      GO TO 50                                                          01800300
2     XINC=XINC*0.5                                                     01800310
      BOT=TOP                                                           01800320
      TOP=BOT+XINC                                                      01800330
      ABOT=ATOP                                                         01800340
      IVAL=IVAL-1                                                       01800350
      IF (IVAL)22,22,21                                                 01800360
22    CONVR2=TOP                                                        01800370
      GO TO 99                                                          01800380
21    ARGLST(1)=TOP                                                     01800390
      ATOP=XNAME(ARGLST)                                                01800400
      GO TO 50                                                          01800410
40    IF (ATOP-ANS)42,41,42                                             01800420
41    CONVR2=TOP                                                        01800430
      GO TO 99                                                          01800440
42    CONVR2=BOT                                                        01800450
99    CONTINUE                                                          01800460
      RETURN                                                            01800470
      END                                                               01800480
      FUNCTION DON1(ARGLST)                                             01900010
C                                                                       01900020
      COMMON  A1,     A2,     AF,     AFH,    ALFA,   BHAL            01900030
      COMMON  AOX,    BESS,   BETAF,  BSQR,   C3P                     01900040
      COMMON  C4P,    CIGN,   CON1,   CSUBP,  DELDI,  DZERO           01900050
      COMMON  EE,     EOX,    ETA,    GAMMA,  GMW,    HDN             01900060
      COMMON  HDP,    IJIM,   IPLOT,  K,      KAP1,   KAP2            01900070
      COMMON  KPF,    EPS,    MOX,    MT,     NP1,    P               01900080
      COMMON  POWD,   POWIGN, PSTART, PSTOP,  QAP,    QEF             01900090
      COMMON  QFUEL,  QL,     QPF,    R,      RAP,    RE              01900100
      COMMON  RHOE,   RHOP,   RHOX,   RON,    SOX,    TAP             01900110
      COMMON  TAV,    TF,     TIT1(20),TZERO, TS                      01900120
      COMMON  XLAMB,  XN1,    XN2,    XN3,    XNU,    XNU1            01900130
      COMMON  XSTAP,  XSTARO, XSTPD,  XSTPF,  XNUP,   ETAP            01900140
      COMMON  PMW,    IPLT,   GAM,    DEL,    XNUU,   WAP             01900150
      COMMON  PR1,    PR2,    PR3,    PR4,    PR6,    PR7             01900160
      COMMON PR8                                                        01900170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)               01900180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                   01900190
      COMMON CZERO,SIGC,CRIT,QSOLID                                     01900200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                             01900210
      COMMON AFH1,ME,XSPD,XSAP,ISI                                      01900220
      COMMON C25(20),NJOB,IJX                                           01900230
      COMMON SII(20),QLIQ                                               01900240
      COMMON INI,M1                                                     01900250
      COMMON QAL                                                        01900260
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1140            C                                                                       01900270
1141                  REAL KAP1,KAP2,KPF,MDX,MT                                         01900280
1142                  REAL MDX1,MDX2                                                    01900290
1143                  INTEGER AH                                                        01900300
1144                  DIMENSION ARGLST(20)                                              01900310
1145                  DIMENSION A(20),B(20),D(20)                                       01900320
1146                  XSPF=XSTPF                                                        01900330
1147                  XSPD=XSTPD                                                        01900340
1148                  TS=ARGLST(1)                                                      01900350
1149                  C3=ARGLST(3)                                                      01900360
1150                  C4=ARGLST(4)                                                      01900370
1151                  RATC=ARGLST(5)                                                    01900380
1152                  XNC=ARGLST(6)                                                     01900390
1153                  C=ARGLST(7)                                                       01900400
1154                  C5P=ARGLST(8)                                                     01900410
1155                  C11=ARGLST(9)                                                     01900420
1156                  IBB=ARGLST(10)                                                    01900430
1157            80    C2P=GAMMA*PMW*TS**.75/82.06                                       01900440
1158                  C15=C2P                                                           01900450
1159                  C3P=2.*C2P*ETAP*AFH1                                              01900460
1160                  C4P=(7.66*C2P)**2/BSQR                                            01900470
1161            82    MDX=ADX*EXP(-EDX/(1.987*TS))                                      01900480
1162                  SQPSI=C2P*C2P/(BSQR*MDX*MDX)                                      01900490
1163                  C20=SQPSI                                                         01900500
1164                  CALL SDXCL(TS,SDX)                                                01900510
1165                  OMEG=SDX*CRIT*1.E-4*RHDX/(GAM*RHOP)                               01900520
1166                  QAP=CSUBP*(TAP-TZERO)+QL-OMEG*QLIQ                                01900530
1167            32    QPF=CSUBP*((TF-TZERO)-GAM*(TAP-TZERO))/GAM+(1.-DEL)*              01900540
1168           &(1.-EPS-GAM)/GAM*QFUEL-DEL*(1.-EPS-GAM)/GAM*QSOLID                      01900550
1169           &+EPS*QAL/GAM-OMEG*GAM*QLIQ                                              01900560
1170                  QPF=CSUBP*(TF-TZERO)+GAM*QL+(1.-EPS-GAM)*(1.-DEL)*QFUEL-DEL       01900570
1171           &*(1.-EPS-GAM)*QSOLID                                                    01900580
1172           &+EPS*QAL-OMEG*QLIQ                                                      01900590
1173                  MT=MDX*SDX/GAM                                                    01900600
1174                  XSTPF=MT/(KPF*P**XN1)                                             01900610
1175                  DUM2=1.+C4P/(MDX**2)                                              01900620
1176                  IF(DUM2.GT.1.0)GO TO 122                                          01900630
1177            121   DUM3=0.5*C4P/(MDX**2)                                             01900640
1178                  GO TO 124                                                         01900650
1179            122   DUM3=SQRT(DUM2)-1.                                                01900660
1180            124   XSTPD=C3P/(MDX*DUM3)                                              01900670
1181                  CALL FLAME(SQPSI,A,IBB,0)                                         01900680
1182                  CALL NEWRAE(XSTPD,A,B,C,D,C2P,XSTAR)                              01900690
1183                  XSTPD=XSTAR*AFH1                                                  01900700
1184            140   CONTINUE                                                          01900710
1185                  XSTAR=MDX/(RATC*P**XNC)                                           01900720
1186            51    BETAF=AFH1*(XSTAR-XSTPF)/XSTPD                                    01900730
1187                  IF(BETAF.GE.1.0) BETAF=1.0                                        01900740
1188                  IF(BETAF.LE.0.0) BETAF=0.0                                        01900750
1189            55    CONTINUE                                                          01900760
1190                  SQPSI= C5P*C5P/(BSQR*MDX*MDX)                                     01900770
1191                  DUM2=1.+C4/(MDX**2)                                               01900780
1192                  IF (DUM2-1.01)10,10,11                                            01900790
1193            11    DUM3=SQRT(DUM2)-1.                                                01900800
1194                  GO TO 91                                                          01900810
1195            10    DUM3=0.5*C4/(MDX**2)                                              01900820
```

```
 91     XSTARD=C3/(MOX*DUM3)                                                   01900830
        IB=IBB                                                                 01900840
        IBB=2                                                                  01900850
        CALL  FLAME(SOPSI,A,IBB,D)                                             01900860
        CALL  NEWPAF(XSTARD,A,B,C11,D,C5P,XSTA)                                01900870
        XSTARD=XSTA*.05                                                        01900880
 130    CONTINUE                                                               01900890
        IBB=IB                                                                 01900900
 95     ZAP=CSUBP*MOX*XSTAP/XLAMB                                              01900910
C       WRITE(6,200) ZAP                                                       01900920
C  200  FORMAT(10X,'ZAP=',E15.8)                                               01900930
 96     ZAT=ZAP+CSUBP*MOX*XSTARD/XLAMB                                         01900940
C       WRITE(6,210) ZAT                                                       01900950
C  210  FORMAT(10X,'ZAT=',E15.8)                                               01900960
C       ZPF=XSTPD+XSTPF                                                        01900970
C       IF(BETAF.LT.1.0) ZPF=XSTAP*AFH1+XSTPF                                  01900980
        ZPF=BETAF*(XSTPD+XSTPF)+(1.-BETAF)*(XSTAP*AFH1+XSTPF)                  01900990
        ZPF=CSUBP*MT/XLAMB*ZPF                                                 01901000
C       WRITE(6,220) ZPF                                                       01901010
C  220  FORMAT(10X,'FOR B<1 ZPF=',E15.8)                                       01901020
 98     PR1=GAM*QL/CSUBP                                                       01901030
        PR2=(1.-EPS-DEL)*(1.-EPS-GAM)/CSUBP*QFUEL                              01901040
        PR3=DEL*(1.-EPS-GAM)/CSUBP*QSOLID                                      01901050
        IF(ZPF.LE.174.5) GO TO 230                                             01901060
        PR4 = 0.0                                                              01901070
        GO TO 235                                                              01901080
  230   PR4=BETAF*QPF/CSUBP*EXP(-ZPF)                                          01901090
  235   PR5=(1.-BETAF)*GAM/CSUBP                                               01901100
        IF(ZAP.LE.174.5) GO TO 240                                             01901110
        PR6 = 0.0                                                              01901120
        GO TO 245                                                              01901130
  240   PR6=PR5*QAP*EXP(-ZAP)                                                  01901140
  245   IF(ZAT.LE.174.5) GO TO 250                                             01901150
        PR7 = 0.0                                                              01901160
        GO TO 255                                                              01901170
  250   PR7=PR5*QFF*EXP(-ZAT)                                                  01901180
  255   PR8=OMEG*GAM*QLIQ/CSUBP                                                01901190
        PR9=EPS*(1.-GAM-EPS)*QAL                                               01901200
        XTS=TZERO-PR1-PR2+PR3+PR4+PR5+PR7+PR8-PR9                              01901210
        XTS=AMAX1(XTS,500.)                                                    01901220
        DON1=ARGLST(1)-XTS                                                     01901230
 100    RETURN                                                                 01901240
        END                                                                    01901250
        SUBROUTINE SOXCL(TS1,SOX1)                                             02000010
C                                                                              02000020
        COMMON  A1,     A2,      AF,        AFH,    ALFA,    RHAL              02000030
        COMMON  AOX,    BESS,    BETAF, BSQR,   C3P                            02000040
        COMMON  C4P,    CIGN,    CON1,      CSUBP,  DFLDI,   DZERO             02000050
        COMMON  EF,     EOX,     ETA,       GAMMA,  GMW,     HDN               02000060
        COMMON  HDP,    IJIM,    IPLOT,     K,      KAP1,    KAP2              02000070
```

CARD NO **** CONTENTS ****

```
      COMMON KPF,    EPS,     MOX,      MT,    NP1,    P              02000080
      COMMON POWD,   POWIGN,  PSTART,   PSTOP, OAP,    OFF            02000090
      COMMON QFUEL,  QL,      QPF,      R,     RAP,    RF             02000100
      COMMON RHOF,   RHOP,    RHOX,     RON,   SOX,    TAP            02000110
      COMMON TAV,    TF,      TITI(20), TZERO, TS                     02000120
      COMMON XLAMB,  XN1,     XN2,      XN3,   XNU,    XNU1           02000130
      COMMON XSTAP,  XSTARD,  XSTPD,    XSTPF, XNUP,   ETAP           02000140
      COMMON PMW,    IPLT,    GAM,      DEL,   XNUU,   WAP            02000150
      COMMON PR1,    PR2,     PR3,      PR4,   PR6,    PR7            02000160
      COMMON PR8                                                      02000170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)             02000180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                                 02000190
      COMMON CZERO,SIGC,CRIT,QSOLID                                   02000200
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20                           02000210
      COMMON AFH1,MF,XSPD,XSAP,ISI                                    02000220
      COMMON C25(20),NJOB,IJX                                         02000230
      COMMON SII(20),QLIO                                             02000240
      COMMON INI,MI                                                   02000250
      COMMON QAL                                                      02000260
C                                                                     02000270
      REAL KAP1,KAP2,KPF,MOX,MT                                       02000280
      RF=RHOF*AF*EXP(-EF/(1.987*TS1))                                 02000290
      RAP=MOX/RHOX                                                    02000300
      RONN=RON*RAP*CIGN                                               02000310
      HDP=A1*(1.-RAP/RF)+RONN                                         02000320
      HDN=A2*(1.-RAP/RF)+RONN                                         02000330
      IF(HDP.GT.0.5)HDP=0.5                                           02000340
      IF(HDP.LT.-0.5)HDP=-0.5                                         02000350
      IF(HDN.GT.0.5)HDN=0.5                                           02000360
      IF(HDN.LT.-0.5)HDN=-0.5                                         02000370
      HDP2=HDP*HDP                                                    02000380
      HDN2=HDN*HDN                                                    02000390
      SOX1=3.*XNUSC*(HDP2+HDN2+1./3.)/(1.+3.*XNUSC                    02000400
     $*(HDP2+HDN2))                                                   02000410
      RETURN                                                          02000420
      END                                                             02000430
      SUBROUTINE NEWRAE(XI,A,B,C,D,C2P,XSTAR)                         02100010
C                                                                     02100020
      COMMON A1,     A2,      AF,       AFH,   ALFA,   RHAL           02100030
      COMMON AOX,    BESS,    BETAF, BSQR,  C3P                       02100040
      COMMON C4P,    CIGN,    CON1,     CSUBP, DELDI,  DZERO          02100050
      COMMON EF,     EOX,     ETA,      GAMMA, GMW,    HDN            02100060
      COMMON HDP,    IJIM,    IPLOT,    K,     KAP1,   KAP2           02100070
      COMMON KPF,    EPS,     MOX,      MT,    NP1,    P              02100080
      COMMON POWD,   POWIGN,  PSTART,   PSTOP, QAP,    OFF            02100090
      COMMON QFUEL,  QL,      QPF,      R,     RAP,    RF             02100100
      COMMON RHOF,   RHOP,    RHOX,     RON,   SOX,    TAP            02100110
      COMMON TAV,    TF,      TITI(20), TZERO, TS                     02100120
      COMMON XLAMB,  XN1,     XN2,      XN3,   XNU,    XNU1           02100130
      COMMON XSTAP,  XSTARD,  XSTPD,    XSTPF, XNUP,   ETAP           02100140
```

```
      COMMON  PMW,    IPLT,    GAM,        DEL,    XNUU,    WAP
      COMMON  PR1,    PR2,     PR3,        PR4,    PR6,     PR7
      COMMON PRP
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)
      COMMON NN,RHOPI,XNUSC,RON1,RONN
      COMMON C7ERO,SIGC,CRIT,QSOLI)
      COMMON SIGSC,IX,LLL,RN,AH,C10,C15,C20
      COMMON AFH1,ME,XSPD,XSAP,ISI
      COMMON C25(20),NJOB,IJX
      COMMON SII(20),QLIO
      COMMON INI,M1
      COMMON QAL
C
      REAL MOX
      DIMENSION A(20),B(20),D(20)
C     WRITE(6,100) C
C 100 FORMAT(10X' C = ',E15.8)
C     WRITE(6,101) XI
C 101 FORMAT(10X'XI = ',E15.8)
      XI=XI*C2P/(MOX*BSQR*AFH1)
      EP=.01E-4*C2P/(MOX*BSQR*AFH1)
      I=0
      NNN=7
      XI=XI*.5
1     SUM2=0.0
      SUM1=0.0
      DO 5 J=1,NNN
      SUM3=A(J)/EXP(D(J)*XI)
      IF(SUM3.LT.1.0E-4)GO TO 6
C     WRITE(6,102) SUM3
C 102 FORMAT(10X'SUM3 = ',E15.8)
      SUM1=SUM1+SUM3
      SUM2=SUM2-A(J)*D(J)/EXP(D(J)*XI)
5     CONTINUE
2     XII=XI-(SUM1-C)/SUM2
      XIX=XII-XI
      XI=XII
      IF(ABS(XIX).LT.EP)GO TO 6
      I=I+1
      XSTAR=XI*MOX*BSQR/C2P
C     WRITE(6,104)I, XSTAR
C 104 FORMAT(10X,I5,' = ',E15.8)
      IF(I.LT.10)GO TO 1
      GO TO 10
6     XSTAR=XI*MOX*BSQR/C2P
10    CONTINUE
      RETURN
      END
      SUBROUTINE FLAME(SQPSI,A,IBB,D)
C
      COMMON  A1,     A2,      AF,         AFH,    ALFA,    RHAL
      COMMON  AOX,    BESS,    BETAF, BSQR,    C3P
      COMMON  C4P,    CIGN,    CON1,       CSUBP, DELDI,   DZERO
      COMMON  EF,     EOX,     ETA,        GAMMA, GMW,     HDN
      COMMON  HDP,    IJIM,    IPLOT,      K,     KAP1,    KAP2
      COMMON  KPF,    EPS,    MOX,        MT,    NP1,     P
```

```
      COMMON  POWD,   POWIGN,  PSTART,  PSTOP, QAP,    QFF          02200090
      COMMON  QFUEL,  QL,      QPF,     R,     RAP,    RF           02200100
      COMMON  RHOF,   RHOP,    RHOX,    RON,   SOX,    TAP          02200110
      COMMON  TAV,    TF,      TITI(20), TZERO, TS                  02200120
      COMMON  XLAMB,  XN1,     XN2,     XN3,   XNU,    XNU1         02200130
      COMMON  XSTAP,  XSTARD,  XSTPD,   XSTPF, XNUP,   ETAP         02200140
      COMMON  PMW,    IPLT,    GAM,     DEL,   XNUU,   WAP          02200150
      COMMON  PR1,    PR2,     PR3,     PR4,   PR6,    PR7          02200160
      COMMON PR8                                                    02200170
      COMMON DMIN(20),DZERO1(20),DMAX(20),SLP(20),SIG(20)           02200180
      COMMON NN,RHOPI,XNUSC,RON1,RONN                               02200190
      COMMON CZERO,SIGC,CRIT,QSOLID                                 02200200
      COMMON SIGSC,IX,LLL,EN,AH,C10,C15,C20                         02200210
      COMMON AEH1,ME,XSPD,XSAP,ISI                                  02200220
      COMMON C25(20),NJOB,IJX                                       02200230
      COMMON SII(20),QLIQ                                           02200240
      COMMON INI,M1                                                 02200250
      COMMON QAL                                                    02200260
C                                                                   02200270
      DIMENSION A(20),D(20)                                         02200280
      DIMENSION ANN(4)                                              02200290
      REAL*8 ANN,ROOT,AUG,DSQPSI,CB,B                               02200300
      DSQPSI=SQPSI                                                  02200310
      DO 5 J=1,9                                                    02200320
      ROOT=BROOT(J)                                                 02200330
      AUG=ROOT*CON1                                                 02200340
      CALL BESSEL(ROOT,AUG,ANN)                                     02200350
      IF(IBB.EQ.2)GO TO 10                                          02200360
      A(J)=ANN(3)/(ANN(1)*ROOT)                                     02200370
      A(J)=-A(J)                                                    02200380
      GO TO 15                                                      02200390
10    A(J)=ANN(3)/(ANN(1)*ANN(1)*ROOT)                              02200400
   15 B=1.D0+4.D0*DSQPSI*ROOT*ROOT                                  02200410
      IF(B.GT.1.0100)GO TO 20                                       02200420
40    IF(IJX.NE.1)GO TO 35                                          02200430
      CB=DSQRT(B)-1.D0                                              02200440
      IJX=0                                                         02200450
      CB=CB/(ROOT*ROOT*DSQPSI)                                      02200460
35    B=CB*ROOT*ROOT*DSQPSI                                         02200470
      GO TO 30                                                      02200480
20    B=DSQRT(B)-1.D0                                               02200490
30    D(J)=B/(2.D0*DSQPSI)                                          02200500
      C25(J)=D(J)                                                   02200510
5     CONTINUE                                                      02200520
C     WRITE(6,100)A                                                 02200530
C     WRITE(6,100)B                                                 02200540
C 100 FORMAT(10X,E15.8)                                             02200550
      RETURN                                                        02200560
      END                                                           02200570
      FUNCTION BROOT(NI)                                            02300010
```

CARD NO	****	CONTENTS	****
1402		GO TO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17),NI	02300020
1403	1	BROOT=3.8317	02300030
1404		RETURN	02300040
1405	2	BROOT=7.0156	02300050
1406		RETURN	02300060
1407	3	BROOT=10.1735	02300070
1408		RETURN	02300080
1409	4	BROOT=13.3237	02300090
1410		RETURN	02300100
1411	5	BROOT=16.4706	02300110
1412		RETURN	02300120
1413	6	BROOT=19.635	02300130
1414		RETURN	02300140
1415	7	BROOT=22.7765	02300150
1416		RETURN	02300160
1417	8	BROOT=25.9181	02300170
1418		RETURN	02300180
1419	9	BROOT=29.0597	02300190
1420		RETURN	02300200
1421	10	BROOT=32.2013	02300210
1422		RETURN	02300220
1423	11	BROOT=33.7573	02300230
1424		RETURN	02300240
1425	12	BROOT=35.3428	02300250
1426		RETURN	02300260
1427	13	BROOT=36.9002	02300270
1428		RETURN	02300280
1429	14	BROOT=38.4845	02300290
1430		RETURN	02300300
1431	15	BROOT=40.0428	02300310
1432		RETURN	02300320
1433	16	BROOT=41.6261	02300330
1434		RETURN	02300340
1435	17	BROOT=43.1853	02300350
1436		RETURN	02300360
1437		END	02300370